

SUPPLEMENTAL DATA 1: MATERIAL IDENTIFICATION

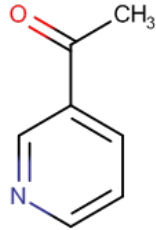
Table 1: Material Identification		
Material	Synonyms	Structure
<p align="center">3-Acetylpyridine</p> <p align="center">C₇H₇NO</p> <p>CAS # 350-03-8</p> <p>Log K_{ow}: 0.49 (EPI Suite)</p> <p>Molecular Weight: 121.13</p> <p>Vapor Pressure: 0.0864 mm Hg @ 20°C: (EPI Suite v4.0)</p> <p>Water Solubility: 42670 mg/L (EPI Suite)</p>	<p>β-Acetylpyridine; 1-(3-Pyridinyl)ethanone</p> <p>1-Pyridin-3-ylethanone</p> <p>3-Acetylpyridine</p> <p>Ethanone, 1-(3-pyridenyl)-</p> <p>Methyl β-pyridyl ketone</p> <p>Methyl 3-pyridyl ketone</p> <p>Methyl pyridyl ketone</p>	

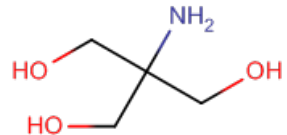
Table 1: Material Identification		
Material	Synonyms	Structure
<p>2-Amino-2-(hydroxymethyl)-1,3-propanediol</p> <p>$C_4H_{11}NO_3$</p> <p>CAS # 77-86-1</p> <p>Log K_{ow}: -1.56 (EPI Suite)</p> <p>Molecular Weight: 121.13</p> <p>Vapor Pressure: 0.000000994 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1e+006 mg/L (EPI Suite)</p>	<p>1,3-Propanediol, 2-amino-2-(hydroxymethyl)-</p> <p>2-Amino-2-(hydroxymethyl)-1,3-propanediol</p> <p>2-Amino-2-(hydroxymethyl)propane-1,3-diol</p> <p>Tham</p> <p>Tris</p> <p>Tris Amino</p> <p>Tris(hydroxymethyl)amino methane</p> <p>Trometamol</p> <p>Tromethamine</p>	

Table 1: Material Identification


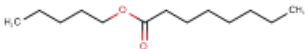
Material	Synonyms	Structure
<p>Amyl formate</p> <p>$C_6H_{12}O_2$</p> <p>CAS # 638-49-3</p> <p>Log K_{ow}: 1.79 (EPI Suite)</p> <p>Molecular Weight: 116.16</p> <p>Vapor Pressure: 7.26 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 3066 mg/L (EPI Suite)</p>	<p>Amyl formate</p> <p>Formic acid, pentyl ester</p> <p>Pentyl formate</p> <p>キ酸アルキル(C=3~5)</p>	
<p>Amyl octanoate</p> <p>$C_{13}H_{26}O_2$</p> <p>CAS # 638-25-5</p> <p>Log K_{ow}: 5.28 (EPI Suite)</p> <p>Molecular Weight: 214.34</p> <p>Vapor Pressure: 0.00938 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1.132 mg/L (EPI Suite)</p>	<p>Amyl caprylate</p> <p>Amyl octanoate</p> <p>Amyl octylate</p> <p>Octanoic acid, pentyl ester</p> <p>Pentyl octanoate</p> <p>Pentyl octylate</p> <p>アルカン酸(C=6~10)アルキル(C=1~10)</p>	

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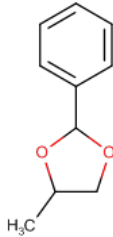
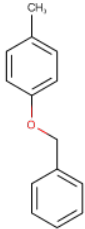
Material	Synonyms	Structure
<p>Benzaldehyde propylene glycol acetal</p> <p>$C_{10}H_{12}O_2$</p> <p>CAS # 2568-25-4</p> <p>Log K_{ow}: 1.74 (EPI Suite)</p> <p>Molecular Weight: 164.2</p> <p>Vapor Pressure: 0.0287 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 2119 mg/L (EPI Suite)</p>	<p>1,3-Dioxolane, 4-methyl-2-phenyl-</p> <p>4-Methyl-2-phenyl-m-dioxolane</p> <p>4-Methyl-2-phenyl-1,3-dioxolane</p> <p>Benzaldehyde propylene glycol acetal</p>	 <p>The structure shows a five-membered 1,3-dioxolane ring with a methyl group (H₃C) at the 4-position and a phenyl ring at the 2-position.</p>
<p>Benzene, 1-methyl-4-(phenylmethoxy)-</p> <p>$C_{14}H_{14}O$</p> <p>CAS # 834-25-3</p> <p>Log K_{ow}: 4.33 (EPI Suite)</p> <p>Molecular Weight: 198.26</p> <p>Vapor Pressure: 0.000848 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 8.972 mg/L (EPI Suite)</p>	<p>Benzene, 1-methyl-4-(phenylmethoxy)-</p> <p>Benzyl 4-methylphenyl ether</p>	 <p>The structure shows a benzene ring with a methyl group (CH₃) at the 4-position and a phenylmethoxy group (-OCH₂Ph) at the 1-position.</p>

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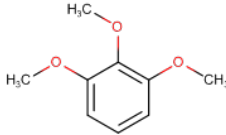
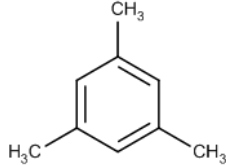
Material	Synonyms	Structure
<p>Benzene, 1,2,3-trimethoxy-</p> <p>$C_9H_{12}O_3$</p> <p>CAS # 634-36-6</p> <p>Log K_{ow}: 1.5 (EPI Suite)</p> <p>Molecular Weight: 168.19</p> <p>Vapor Pressure: 0.0202 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 3096 mg/L (EPI Suite)</p>	<p>Benzene, 1,2,3-trimethoxy-</p>	 <p>The structure shows a benzene ring with three methoxy groups (-OCH₃) attached at the 1, 2, and 3 positions. The methoxy groups are shown as H₃C-O-CH₃ groups.</p>
<p>Benzene, 1,3,5-trimethyl-</p> <p>C_9H_{12}</p> <p>CAS # 108-67-8</p> <p>Log K_{ow}: 3.63 (EPI Suite)</p> <p>Molecular Weight: 120.19</p> <p>Vapor Pressure: 1.43 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 120.3 mg/L (EPI Suite)</p>	<p>Benzene, 1,3,5-trimethyl-</p>	 <p>The structure shows a benzene ring with three methyl groups (-CH₃) attached at the 1, 3, and 5 positions.</p>

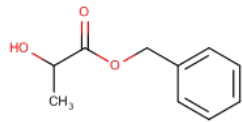
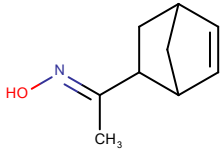
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Benzyl 2-hydroxypropionate</p> <p>C₁₀H₁₂O₃</p> <p>CAS # 2051-96-9</p> <p>Log K_{ow}: 1.03 (EPI Suite)</p> <p>Molecular Weight: 180.2</p> <p>Vapor Pressure: 0.00013 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility 23290 mg/L (EPI Suite)</p>	<p>Benzyl 2-hydroxypropanoate</p> <p>Benzyl 2-hydroxypropionate</p> <p>Benzyl lactate</p> <p>Phenylmethyl 2-hydroxypropanoate</p> <p>Propanoic acid, 2-hydroxy-, phenylmethyl ester</p>	
<p>1-Bicyclo[2.2.1]hept-5-en-2-ylethan-1-one-oxime</p> <p>C₉H₁₃NO</p> <p>CAS # 65416-21-9</p> <p>Log K_{ow}: 3.15 (EPI Suite)</p> <p>Molecular Weight: 151.2</p> <p>Vapor Pressure: 0.001 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 154.1 mg/L (EPI Suite)</p>	<p>1-Bicyclo[2.2.1]hept-5-en-2-ylethan-1-one-oxime</p> <p>1-Bicyclo[2.2.1]hept-5-en-2-ylethanone oxime</p> <p>2-(1-Oximidoethyl)bicyclo[2.2.1]hept-5-ene</p> <p>Ethanone, 1-bicyclo[2.2.1]hept-5-en-2-yl-, oxime</p> <p>Terravert</p>	

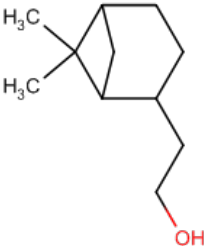
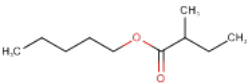
Table 1: Material Identification		
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<p>Bicyclo[3.1.1]heptane-2-ethanol,6,6-dimethyl-</p> <p>C₁₁H₂₀O</p> <p>CAS # 4747-61-9</p> <p>Log K_{ow}:3.38 (EPI Suite)</p> <p>Molecular Weight: 168.28</p> <p>Vapor Pressure: 0.00175mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility:263.2 mg/L (EPI Suite)</p>	<p>6,6-Dimethylbicyclo[3.1.1]heptane-2-ethanol</p> <p>Bicyclo[3.1.1]heptane-2-ethanol, 6,6-dimethyl-</p> <p>Dihydrohomomyrtenol</p>	
<p>Butanoic acid, 2-methyl-, pentyl ester</p> <p>C₁₁H₂₀O₂</p> <p>CAS # 68039-26-9</p> <p>Log K_{ow}: 3.74 (EPI Suite)</p> <p>Molecular Weight: 172.26</p> <p>Vapor Pressure: 0.259 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 38.59 mg/L (EPI Suite)</p>	<p>Butanoic acid, 2-methyl-, pentyl ester</p> <p>Pentyl 2-methylbutyrate</p>	

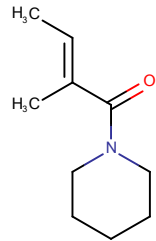
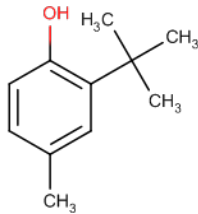
Table 1: Material Identification		
Material	Synonyms	Structure
<p>2-Buten-1-one, 2-methyl-1-(1-piperidinyl)-</p> <p>C₁₀H₁₇NO</p> <p>CAS # 54533-29-8</p> <p>Log K_{ow}: 2.19 (EPI Suite)</p> <p>Molecular Weight: 167.25</p> <p>Vapor Pressure: 0.00404 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 853.4 mg/L (EPI Suite)</p>	<p>2-Buten-1-one, 2-methyl-1-(1-piperidinyl)-</p> <p>Piperidine, 1-(2-methyl-1-oxo-2-butenyl)-</p>	
<p>2-tert-Butyl-p-cresol</p> <p>C₁₁H₁₆O</p> <p>CAS # 2409-55-4</p> <p>Log K_{ow}: 3.97 (EPI Suite)</p> <p>Molecular Weight: 164.24</p> <p>Vapor Pressure: 0.00727 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 101.3 mg/L (EPI Suite)</p>	<p>2-(1,1-Dimethylethyl)-4-methylphenol</p> <p>2-tert-Butyl-p-cresol</p> <p>2-tert-Butyl-4-methylphenol</p> <p>Phenol, 2-(1,1-dimethylethyl)-4-methyl-</p>	

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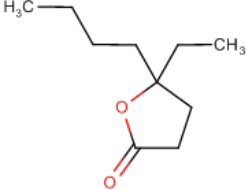

Material	Synonyms	Structure
<p>5-Butyl-5-ethylidihydrofuran-2(3H)-one</p> <p>$C_{10}H_{18}O_2$</p> <p>CAS # 68188-98-7</p> <p>Log K_{ow}: 2.53 (EPI Suite)</p> <p>Molecular Weight: 170.25</p> <p>Vapor Pressure: 0.00407 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 424 mg/L (EPI Suite)</p>	<p>2(3H)-Furanone, 5-butyl-5-ethylidihydro-</p> <p>4-Ethyl-4-hydroxyoctanoicacid lactone</p> <p>5-Butyl-5-ethylidihydrofuran-2(3H)-one</p> <p>Decalactone</p>	
<p>Butyl formate</p> <p>$C_5H_{10}O_2$</p> <p>CAS # 592-84-7</p> <p>Log K_{ow}: 1.3 (EPI Suite)</p> <p>Molecular Weight: 102.13</p> <p>Vapor Pressure: 21.9 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 8958 mg/L (EPI Suite)</p>	<p>Butyl formate</p> <p>Butyl methanoate</p> <p>Formic acid, butyl ester</p>	

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Material	Synonyms	Structure
<p>Butyl hexanoate</p> <p>$C_{10}H_{20}O_2$</p> <p>CAS # 626-82-4</p> <p>Log K_{ow}: 3.81 (EPI Suite)</p> <p>Molecular Weight: 172.26</p> <p>Vapor Pressure: 0.162 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 33.39 mg/L (EPI Suite)</p>	<p>Butyl caproate</p> <p>Butyl hexanoate</p> <p>Hexanoic acid, butyl ester</p> <p>アルカン酸(C=6~10)アルキル(C=1~10)</p>	
<p>Butyl isobutyrate</p> <p>$C_8H_{16}O_2$</p> <p>CAS # 97-87-0</p> <p>Log K_{ow}: 2.76 (EPI Suite)</p> <p>Molecular Weight: 144.21</p> <p>Vapor Pressure: 2.28 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 356.7 mg/L (EPI Suite)</p>	<p>Butyl 2-methylpropanoate</p> <p>Butyl isobutyrate</p> <p>Propanoic acid, 2-methyl-, butyl ester</p>	

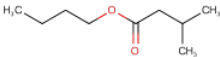
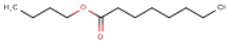
Table 1: Material Identification		
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<p>Butyl isovalerate</p> <p>C₉H₁₈O₂</p> <p>CAS # 109-19-3</p> <p>Log K_{ow}: 3.25 (EPI Suite)</p> <p>Molecular Weight: 158.24</p> <p>Vapor Pressure: 0.726 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 117.8 mg/L (EPI Suite)</p>	<p><i>n</i>-Butyl isovalerate</p> <p>Butanoic acid, 3-methyl-, butyl ester</p> <p>Butyl 3-methylbutanoate</p> <p>Butyl isopentanoate</p> <p>Butyl isovalerate</p> <p>Butyl isovalerianate</p> <p>ヘンタン酸アルキル(C=1~5)</p>	
<p>Butyl octanoate</p> <p>C₁₂H₂₄O₂</p> <p>CAS # 589-75-3</p> <p>Log K_{ow}: 4.79 (EPI Suite)</p> <p>Molecular Weight: 200.32</p> <p>Vapor Pressure: 0.0221 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 3.517 mg/L (EPI Suite)</p>	<p>Butyl caprylate</p> <p>Butyl octanoate</p> <p>Octanoic acid, butyl ester</p> <p>アルカン酸(C=6~10)アルキル(C=1~10)</p>	

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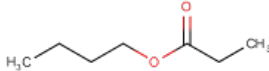
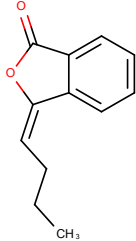
Material	Synonyms	Structure
<p>Butyl propionate</p> <p>$C_7H_{14}O_2$</p> <p>CAS # 590-01-2</p> <p>Log K_{ow}: 2.34 (EPI Suite)</p> <p>Molecular Weight: 130.18</p> <p>Vapor Pressure: 3.37 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 925.9 mg/L (EPI Suite)</p>	<p><i>n</i>-Butyl propionate</p> <p>Butyl propanoate</p> <p>Butyl propionate</p> <p>Propanoic acid, butyl ester</p> <p>プロピオン酸アルキル(C=1~12)</p>	 <p>The structure shows a propionic acid chain (CH3-CH2-C(=O)-) esterified to a butyl group (CH2-CH2-CH2-CH3). The ester oxygen is highlighted in red.</p>
<p>3-Butylidenephthalide</p> <p>$C_{12}H_{12}O_2$</p> <p>CAS # 551-08-6</p> <p>Log K_{ow}: 2.52 (EPI Suite)</p> <p>Molecular Weight: 188.22</p> <p>Vapor Pressure: 0.0000609 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 353.5 mg/L (EPI Suite)</p>	<p>1(3H)-Isobenzofuranone, 3-butylidene-</p> <p>3-Butylidene-2-benzofuran-1(3H)-one</p> <p>3-Butylidenephthalide</p> <p>Butylidene phthalide</p> <p>Ligusticum lactone</p>	 <p>The structure shows a benzofuranone ring system with a butylidene group (-CH=CH-CH2-CH3) attached to the 3-position. The carbonyl oxygen and the ring oxygen are highlighted in red.</p>

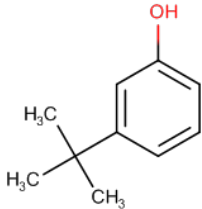
Table 1: Material Identification		
Material	Synonyms	Structure
<p>3-<i>tert</i>-Butylphenol</p> <p>C₁₀H₁₄O</p> <p>CAS # 585-34-2</p> <p>Log K_{ow}: 3.42 (EPI Suite)</p> <p>Molecular Weight: 150.22</p> <p>Vapor Pressure: 0.00754 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 437.4 mg/L (EPI Suite)</p>	<p>3-<i>tert</i>-Butylphenol</p> <p>Phenol, 3-(1,1-dimethylethyl)-</p>	

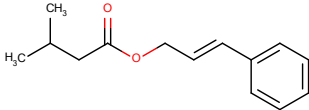
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Cinnamyl isovalerate</p> <p>C₁₄H₁₈O₂</p> <p>CAS # 140-27-2</p> <p>Log K_{ow}: 4.25 (EPI Suite)</p> <p>Molecular Weight: 218.29</p> <p>Vapor Pressure: 0.00115 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 8.282 mg/L (EPI Suite)</p>	<p>3-Phenyl-2-propen-1-yl 3-methylbutanoate</p> <p>3-Phenylallyl 3-methylbutanoate</p> <p>3-Phenylallyl isovalerate</p> <p>3-Phenylprop-2-en-1-yl 3-methylbutanoate</p> <p>Butanoic acid, 3-methyl-, 3-phenyl-2-propenyl ester</p> <p>Cinnamyl 3-methylbutanoate</p> <p>Cinnamyl isovalerate</p> <p>アルカン酸(C=1~6)シナミル</p>	

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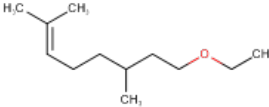
Material	Synonyms	Structure
<p data-bbox="464 321 741 345">Citronellyl ethyl ether</p> <p data-bbox="548 380 657 404">C₁₄H₁₈O₂</p> <p data-bbox="243 565 468 589">CAS # 69929-16-4</p> <p data-bbox="243 686 541 711">Log K_{ow}: 4.75 (EPI Suite)</p> <p data-bbox="243 743 548 768">Molecular Weight: 184.32</p> <p data-bbox="243 800 905 824">Vapor Pressure: 0.171 mm Hg @ 20°C (EPI Suite v4.0)</p> <p data-bbox="243 857 575 881">Water Solubility: (EPI Suite)</p>	<p data-bbox="1052 532 1440 557">2-Octene, 8-ethoxy-2,6-dimethyl-</p> <p data-bbox="1062 589 1430 613">8-Ethoxy-2,6-dimethyl-2-octene</p> <p data-bbox="1121 654 1371 678">Citronellyl ethyl ether</p>	 <p>The chemical structure shows a branched alkene chain with an ethoxy group. The chain starts with a double bond between carbons 2 and 3. Carbon 2 has a methyl group (CH₃) and a hydrogen atom (H₃C) attached. Carbon 3 has a hydrogen atom (H) and a hydrogen atom (H) attached. The chain continues to carbon 6, which has a methyl group (CH₃) attached. Carbon 7 is bonded to carbon 6 and carbon 8. Carbon 8 is bonded to carbon 7 and an oxygen atom (O). The oxygen atom is bonded to an ethyl group (CH₂CH₃).</p>

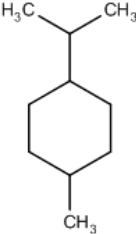
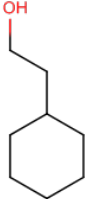
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Cyclohexane, 1-methyl-4-(1-methylethyl)-</p> <p>C₁₀ H₂₀</p> <p>CAS # 99-82-1</p> <p>Log K_{ow}: 4.92 (EPI Suite)</p> <p>Molecular Weight: 140.27</p> <p>Vapor Pressure: 1.24 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 0.4331 mg/L (EPI Suite)</p>	<p>1-Isopropyl-4-methylcyclohexane</p> <p>Cyclohexane, 1-methyl-4-(1-methylethyl)</p>	
<p>2-Cyclohexylethyl alcohol</p> <p>C₈H₁₆O</p> <p>CAS # 4442-79-9</p> <p>Log K_{ow}: 2.62</p> <p>Molecular Weight: 128.21</p> <p>Vapor Pressure: 0.028 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1752 mg/L (EPI Suite)</p>	<p>2-Cyclohexylethanol</p> <p>2-Cyclohexylethyl alcohol</p> <p>Cyclohexaneethanol</p> <p>Cyclohexylethanol</p> <p>Cyclohexylethyl alcohol</p> <p>Hexahydrophenylethyl alcohol</p>	

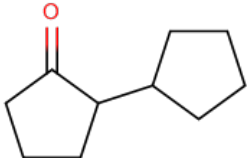
Table 1: Material Identification		
Material	Synonyms	Structure
<p>2-Cyclopentylcyclopentanone</p> <p>C₁₀H₁₆O</p> <p>CAS # 4884-24-6</p> <p>Log K_{ow}: 2.83 (EPI Suite)</p> <p>Molecular Weight: 152.23</p> <p>Vapor Pressure: 0.0513 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 283.6 mg/L (EPI Suite)</p>	<p>[1,1'-Bicyclopentyl]-2-one</p> <p>1,1'-Bi(cyclopentyl)-2-one</p> <p>1,1'-Bi(cyclopentyl)-2-one</p> <p>2-Cyclopentylcyclopentanone</p>	

Table 1: Material Identification

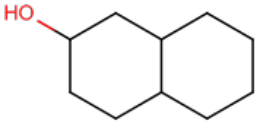
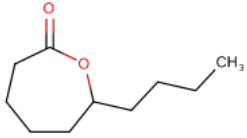
Material	Synonyms	Structure
<p>Decahydro-β-naphthol</p> <p>C₁₀H₁₈O</p> <p>CAS # 825-51-4</p> <p>Log K_{ow}: 2.66 (EPI Suite)</p> <p>Molecular Weight: 154.25</p> <p>Vapor Pressure: 0.00354 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1263 mg/L (EPI Suite)</p>	<p><i>trans</i>-Decahydro-β-naphthol</p> <p>2-Decalol</p> <p>2-Naphthalenol, decahydro-</p> <p>Decahydro-β-naphthol</p> <p>Decahydro-2-naphthol</p> <p>Decahydronaphthalen-2-ol</p>	
<p>ε-Decalactone</p> <p>C₁₀H₁₈O₂</p> <p>CAS # 5579-78-2</p> <p>Log K_{ow}: 2.57 (EPI Suite)</p> <p>Molecular Weight: 170.25</p> <p>Vapor Pressure: 0.00272 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 393.8 mg/L (EPI Suite)</p>	<p>ε-Decalactone</p> <p>2-Oxepanone, 7-butyl-</p> <p>6-Butylhexanolide</p> <p>7-Butyl-2-oxepanone</p> <p>7-Butyloxepan-2-one</p>	

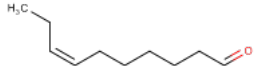
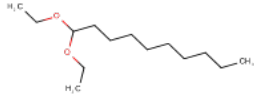
Table 1: Material Identification		
Material	Synonyms	Structure
<p>7-Decenal, (7Z)-</p> <p>C₁₀H₁₈O</p> <p>CAS # 21661-97-2</p> <p>Log K_{ow}: 3.55 (EPI Suite)</p> <p>Molecular Weight: 154.25</p> <p>Vapor Pressure: 0.119 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 67.8 mg/L (EPI Suite)</p>	<p>(<i>cis</i>)-7-Decen-1-al</p> <p>7-Decenal, (7Z)-</p>	
<p>1,1-Diethoxydecane</p> <p>C₁₄H₃₀O₂</p> <p>CAS # 34764-02-8</p> <p>Log K_{ow}: 5.13 (EPI Suite)</p> <p>Molecular Weight: 230.39</p> <p>Vapor Pressure: 0.017 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 1.25 mg/L (EPI Suite)</p>	<p>1,1-Bis(ethoxy)decane</p> <p>1,1-Diethoxydecane</p> <p>Caprylaldehyde diacetal</p> <p>Decanal diethyl acetal</p> <p>Decane, 1,1-diethoxy-</p> <p>Decylaldehyde diethyl acetal</p>	

Table 1: Material Identification		
Material	Synonyms	Structure
<p>(2Z,6Z)-1,1-Diethoxynona-2,6-diene*</p> <p>C₁₃H₂₄O₂</p> <p>CAS # 67674-37-7</p> <p>Log K_{ow}: 4.21 (EPI Suite)</p> <p>Molecular Weight: 212.33</p> <p>Vapor Pressure: 0.0151 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 9.542 mg/L (EPI Suite)</p> <p>*Additional Material for Main CAS # 67674-36-6</p>	<p>(2Z,6Z)-1,1-Diethoxynona-2,6-diene</p> <p>1,1-Diethoxynona-2,6-diene</p> <p>2,6-Nonadiene, 1,1-diethoxy-, (Z,Z)-</p> <p>2(Z)-6(Z)-Nonadienal diethyl acetal</p>	

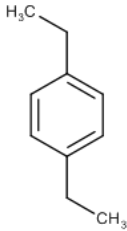
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Diethylbenzene</p> <p>C₁₀H₁₄</p> <p>CAS # 25340-17-4</p> <p>Log K_{ow}: 4.07 (EPI Suite)</p> <p>Molecular Weight: 134.22</p> <p>Vapor Pressure: 0.638 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 10.85 mg/L (EPI Suite)</p>	<p>1,2-Diethylbenzene</p> <p>Benzene, diethyl-</p> <p>Diethylbenzene</p>	

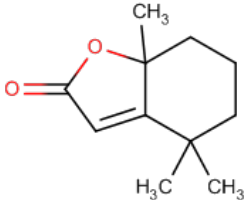
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Dihydroactinidiolide*</p> <p>C₁₁H₁₆O₂</p> <p>CAS # 17092-92-1</p> <p>Log K_{ow}: 2.3 (EPI Suite)</p> <p>Molecular Weight: 180.24</p> <p>Vapor Pressure: 0.00177 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 600.6 mg/L (EPI Suite)</p> <p>*Additional Material for Main CAS # 15356-74-8</p>	<p>2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro- 4,4,7a-trimethyl-, (R)- Dihydroactinidiolide</p>	

Table 1: Material Identification

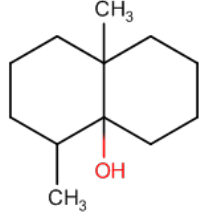
Material	Synonyms	Structure
<p>1,10-Dimethyl-9-decalol*</p> <p>C₁₂H₂₂O</p> <p>CAS # 19700-21-1</p> <p>Log K_{ow}: 3.57 (EPI Suite)</p> <p>Molecular Weight: 182.32</p> <p>Vapor Pressure: 0.00057 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 156.7 mg/L (EPI Suite)</p> <p>*Additional Material for Main CAS # 23333-91-7</p>	<p>1,10-Dimethyl-9-decalol</p> <p>4,8a-Dimethyloctahydronaphthalen-4a(2H)-ol</p> <p>4a(2H)-Naphthalenol, octahydro-4,8a-dimethyl-, [(4α,4α,8aβ)]-</p> <p>Geosmin</p>	 <p>The chemical structure is a decalin derivative. It consists of two fused six-membered rings. At the top bridgehead position (C1), there is a methyl group (CH₃). At the bottom bridgehead position (C10), there is another methyl group (CH₃). At the C9 position, which is adjacent to both bridgeheads, there is a hydroxyl group (OH) shown in red.</p>

Table 1: Material Identification

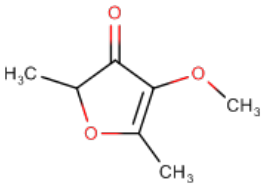
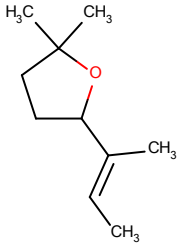
Material	Synonyms	Structure
<p>2,5-Dimethyl-4-methoxy-3(2H)-furanone</p> <p>$C_7H_{10}O_3$</p> <p>CAS # 4077-47-8</p> <p>Log K_{ow}: 0.62 (EPI Suite)</p> <p>Molecular Weight: 142.15</p> <p>Vapor Pressure: 0.132 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 24410 mg/L (EPI Suite)</p>	<p>2,5-Dimethyl-4-methoxy-3(2H)-furanone</p> <p>3(2H)-Furanone, 4-methoxy-2,5-dimethyl-</p> <p>4-Methoxy-2,5-dimethyl-3(2H)-furanone</p> <p>4-Methoxy-2,5-dimethylfuran-3(2H)-one</p>	 <p>The structure shows a five-membered furanone ring. The oxygen atom is at the bottom. A carbonyl group (C=O) is at the top. A methoxy group (-OCH3) is attached to the carbon at the 4-position. Two methyl groups (-CH3) are attached to the carbons at the 2 and 5 positions.</p>
<p>2,2-Dimethyl-5-(1-methylpropen-1-yl)tetrahydrofuran</p> <p>$C_{10}H_{18}O$</p> <p>CAS # 7416-35-5</p> <p>Log K_{ow}: 3.54 (EPI Suite)</p> <p>Molecular Weight: 154.25</p> <p>Vapor Pressure: 1.19 mm Hg @ 25°C (EPI Suite v4.0)</p> <p>Water Solubility: 68.88 mg/L (EPI Suite)</p>	<p>2,2-Dimethyl-5-(1-methylprop-1-en-1-yl)tetrahydrofuran</p> <p>2,2-Dimethyl-5-(1-methylpropen-1-yl)tetrahydrofuran</p> <p>Furan, tetrahydro-2,2-dimethyl-5-(1-methyl-1-propenyl)-</p> <p>Ocimen quintoxide</p>	 <p>The structure shows a five-membered tetrahydrofuran ring. The oxygen atom is at the top. Two methyl groups (-CH3) are attached to the carbon at the 2-position. A 1-methylprop-1-en-1-yl group is attached to the carbon at the 5-position.</p>

Table 1: Material Identification

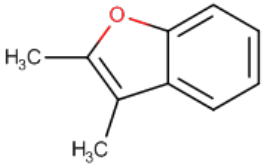
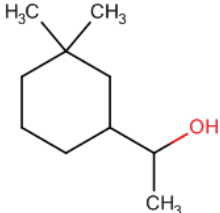
Material	Synonyms	Structure
<p>2,3-Dimethylbenzofuran</p> <p>C₁₀H₁₀O</p> <p>CAS # 3782-00-1</p> <p>Log K_{ow}: 3.63 (EPI Suite)</p> <p>Molecular Weight: 146.18</p> <p>Vapor Pressure: 0.026 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 62.2 mg/L (EPI Suite)</p>	<p>2,3-Dimethyl-1-benzofuran</p> <p>2,3-Dimethylbenzofuran</p> <p>Benzofuran, 2,3-dimethyl-</p>	 <p>The structure shows a benzofuran ring system with two methyl groups (H₃C) attached to the 2 and 3 positions of the furan ring.</p>
<p>1-(3,3-Dimethylcyclohexyl)ethanol</p> <p>C₁₀H₂₀O</p> <p>CAS # 25225-09-6</p> <p>Log K_{ow}: 3.42 (EPI Suite)</p> <p>Molecular Weight: 56.26</p> <p>Vapor Pressure: 0.0187 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 278 mg/L (EPI Suite)</p>	<p>α,3,3-Trimethylcyclohexanemethanol</p> <p>α,3,3-Trimethylcyclohexylmethanol</p> <p>1-(3,3-Dimethylcyclohexyl)ethanol</p> <p>3,3-Dimethylcyclohexyl methyl carbinol</p> <p>Cyclohexanemethanol, α,3,3-trimethyl-</p>	 <p>The structure shows a cyclohexane ring with two methyl groups (H₃C and CH₃) attached to the 3-position. A 1-hydroxyethyl group (CH(OH)CH₃) is attached to the 1-position of the ring.</p>

Table 1: Material Identification

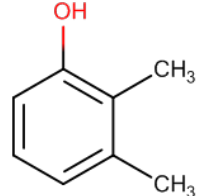
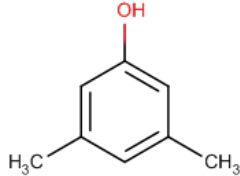
Material	Synonyms	Structure
<p>2,3-Dimethylphenol</p> <p>$C_7H_{10}O_3$</p> <p>CAS # 526-75-0</p> <p>Log K_{ow}: 2.61 (EPI Suite)</p> <p>Molecular Weight: 122.16</p> <p>Vapor Pressure: 0.0137 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 2855 mg/L (EPI Suite)</p>	<p>2,3-Dimethylphenol</p> <p>2,3-Xylenol</p> <p>Phenol, 2,3-dimethyl-</p>	
<p>3,5-Dimethylphenol</p> <p>$C_8H_{10}O$</p> <p>CAS # 108-68-9</p> <p>Log K_{ow}: 2.61 (EPI Suite)</p> <p>Molecular Weight: 122.16</p> <p>Vapor Pressure: 0.013 mm HG @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 3687 mg/L (EPI Suite)</p>	<p>3,5-Dimethylphenol</p> <p>3,5-Xylenol</p> <p>Phenol, 3,5-dimethyl-</p>	

Table 1: Material Identification

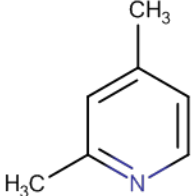
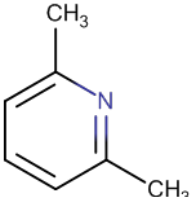
Material	Synonyms	Structure
<p data-bbox="470 321 737 345">2,4-Dimethylpyridine</p> <p data-bbox="562 380 644 404">C₇H₉N</p> <p data-bbox="243 501 436 526">CAS # 108-47-4</p> <p data-bbox="243 623 527 647">Log K_{ow}: 1.9 (EPI Suite)</p> <p data-bbox="243 683 548 708">Molecular Weight: 107.15</p> <p data-bbox="243 743 884 768">Vapor Pressure: 1.92 mm Hg @ 20°C (EPI Suite v4.0)</p> <p data-bbox="243 803 722 828">Water Solubility: 52980 mg/L (EPI Suite)</p>	<p data-bbox="1121 472 1367 496">α,γ-Dimethylpyridine</p> <p data-bbox="1121 532 1367 557">2,4-Dimethylpyridine</p> <p data-bbox="1173 592 1314 617">2,4-Lutidine</p> <p data-bbox="1113 652 1377 677">Pyridine, 2,4-dimethyl-</p>	 <p>The structure shows a pyridine ring with a nitrogen atom at the bottom. Methyl groups (CH₃) are attached to the 2 and 4 positions of the ring. The 2-position methyl group is labeled H₃C and the 4-position methyl group is labeled CH₃.</p>
<p data-bbox="470 872 737 896">2,6-Dimethylpyridine</p> <p data-bbox="562 930 644 954">C₇H₉N</p> <p data-bbox="243 1052 436 1076">CAS # 108-48-5</p> <p data-bbox="243 1174 527 1198">Log K_{ow}: 1.9 (EPI Suite)</p> <p data-bbox="243 1234 548 1258">Molecular Weight: 107.15</p> <p data-bbox="243 1294 884 1318">Vapor Pressure: 3.83 mm Hg @ 20°C (EPI Suite v4.0)</p> <p data-bbox="243 1354 722 1378">Water Solubility: 81510 mg/L (EPI Suite)</p>	<p data-bbox="1121 1084 1367 1109">2,6-Dimethylpyridine</p> <p data-bbox="1173 1144 1314 1169">2,6-Lutidine</p>	 <p>The structure shows a pyridine ring with a nitrogen atom at the top-right. Methyl groups (CH₃) are attached to the 2 and 6 positions of the ring. The 2-position methyl group is labeled CH₃ and the 6-position methyl group is labeled CH₃.</p>

Table 1: Material Identification

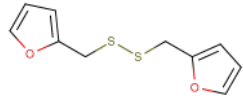
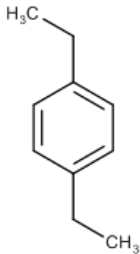
Material	Synonyms	Structure
<p>2,2'-(Dithiodimethylene)-difuran</p> <p>$C_{10}H_{10}O_2S_2$</p> <p>CAS # 4437-20-1</p> <p>Log K_{ow}: 4.03 (EPI Suite)</p> <p>Molecular Weight: 226.31</p> <p>Vapor Pressure: 0.000445 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 11.56 mg/L (EPI Suite)</p>	<p>2-Furfuryl disulfide</p> <p>2,2'-(Dithiodimethylene)-difuran</p> <p>2,2'-[Disulfaneyldibis(methylene)]difuran</p> <p>Bis(2-furfuryl)disulfide</p> <p>Difurfuryl disulfide</p> <p>Furan, 2,2'-[dithiobis(methylene)]bis-</p> <p>Robustone</p>	 <p>The structure shows two furan rings connected by a disulfide bridge (-S-S-) at their 2-positions. Each furan ring is represented as a five-membered ring with one oxygen atom and two double bonds.</p>
<p>3-Dodecyldihydrofuran-2(3H)-one</p> <p>$C_{16}H_{30}O_2$</p> <p>CAS # 73263-36-2</p> <p>Log K_{ow}: 5.51 (EPI Suite)</p> <p>Molecular Weight: 254.41</p> <p>Vapor Pressure: 0.0000144 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 0.4371 mg/L (EPI Suite)</p>	<p>1,2-Diethylbenzene</p> <p>Benzene, diethyl-</p> <p>Diethylbenzene</p>	 <p>The structure shows a benzene ring with two ethyl groups (-CH2CH3) attached at the 1 and 2 positions. The ethyl groups are drawn as lines extending from the ring to a CH2 group, which is then connected to a CH3 group.</p>

Table 1: Material Identification

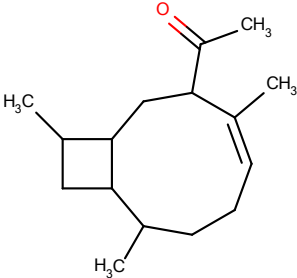
Material	Synonyms	Structure
<p data-bbox="268 321 934 407">Ethanone, 1-(4,11,11,-trimethyl-8-methylenebicyclo[7.2.0]undec-4-enyl)-[1R-(1a,4E,9b)]</p> <p data-bbox="548 440 657 467">C₁₆H₂₆O₁</p> <p data-bbox="243 561 468 589">CAS # 70801-04-6</p> <p data-bbox="243 683 541 711">Log K_{ow}: 4.71 (EPI Suite)</p> <p data-bbox="243 743 548 771">Molecular Weight: 234.38</p> <p data-bbox="243 803 947 831">Vapor Pressure: 0.000589 mm Hg @ 20°C (EPI Suite v4.0)</p> <p data-bbox="243 863 716 891">Water Solubility: 2.716 mg/L (EPI Suite)</p>	<p data-bbox="995 428 1495 581">Ethanone, 1-(4,11,11,-trimethyl-8-methylenebicyclo[7.2.0]undec-4-enyl)-[1R-(1a,4E,9b)]</p> <p data-bbox="995 613 1495 701">Ethanone, 1-[(1R,4E,9R)-4,11,11-trimethyl-8-methylenebicyclo[7.2.0]undec-4-enyl]-</p>	 <p>The chemical structure shows a bicyclic system consisting of a four-membered ring fused to a ten-membered ring. The four-membered ring has a methyl group (H₃C) attached to one of its carbons. The ten-membered ring has a double bond and a methyl group (CH₃) attached to one of its carbons. A carbonyl group (C=O) is attached to the ten-membered ring, with a methyl group (CH₃) attached to the carbonyl carbon. The oxygen atom is shown in red.</p>

Table 1: Material Identification

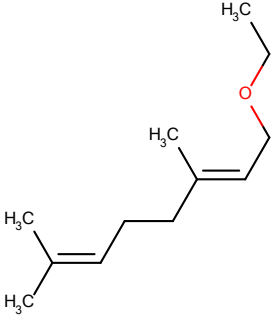
Material	Synonyms	Structure
<p data-bbox="352 321 852 347">(E)-1-Ethoxy-3,7-dimethylocta-2,6-diene</p> <p data-bbox="558 380 655 406">C₁₂H₂₂O</p> <p data-bbox="247 500 466 526">CAS # 22882-91-3</p> <p data-bbox="247 623 541 649">Log K_{ow}: 4.66 (EPI Suite)</p> <p data-bbox="247 682 533 708">Molecular Weight: 182.3</p> <p data-bbox="247 740 915 766">Vapor Pressure: 0.0934 mm Hg @ 20°C (EPI Suite v4.0)</p> <p data-bbox="247 799 714 824">Water Solubility: 5.618 mg/L (EPI Suite)</p> <p data-bbox="247 922 806 948">*Additional Material for Main CAS # 40267-72-9</p>	<p data-bbox="1012 500 1482 526">(E)-1-Ethoxy-3,7-dimethylocta-2,6-diene</p> <p data-bbox="1020 558 1474 584">trans-3,7-Dimethyl-2,6-octadienyl ethyl</p> <p data-bbox="1213 617 1281 643">ether</p> <p data-bbox="1033 682 1461 708">1-Ethoxy-3,7-dimethylocta-2,6-diene</p> <p data-bbox="995 740 1499 766">2,6-Octadiene, 1-ethoxy-3,7-dimethyl-, (E)-</p>	

Table 1: Material Identification		
Material	Synonyms	Structure
<p>(Z)1-Ethoxy-3,7-dimethylocta-2,6-diene</p> <p>C₁₂H₂₂O</p> <p>CAS # 22882-89-9</p> <p>Log K_{ow}: 4.66 (EPI Suite)</p> <p>Molecular Weight: 182.3</p> <p>Vapor Pressure: 0.0934 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 5.618 mg/L (EPI Suite)</p> <p>*Additional Material for Main CAS # 40267-72-9</p>	<p>(Z)1-Ethoxy-3,7-dimethylocta-2,6-diene</p> <p>1-Ethoxy-3,7-dimethylocta-2,6-diene</p> <p>2,6-Octadiene, 1-ethoxy-3,7-dimethyl-, (Z)-</p> <p>Ethyl neryl ether</p>	

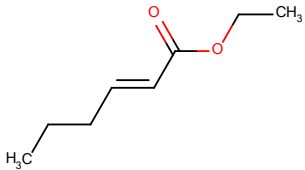
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Ethyl 2-hexenoate</p> <p>$C_8H_{14}O_2$</p> <p>CAS # 1552-67-6</p> <p>Log K_{ow}: 2.61 (EPI Suite)</p> <p>Molecular Weight: 142.19</p> <p>Vapor Pressure: 1.26 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 480.5 mg/L (EPI Suite)</p> <p>*Additional Material for Main CAS # 27829-72-7</p>	<p>2-Hexenoic acid, ethyl ester</p> <p>Ethyl 2-hexenoate</p> <p>Ethyl hex-2-enoate</p>	 <p>The image shows the skeletal structure of ethyl 2-hexenoate. It consists of a six-carbon chain with a double bond between the second and third carbons. The second carbon is also part of an ester group, which is bonded to an ethyl group (CH₂CH₃). The first carbon of the chain is a methyl group (H₃C).</p>

Table 1: Material Identification

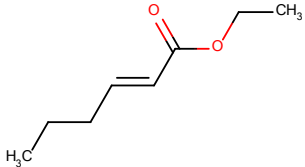
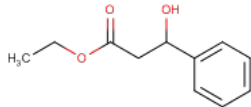
Material	Synonyms	Structure
<p data-bbox="449 321 753 345">Ethyl <i>trans</i>-2-hexenoate</p> <p data-bbox="554 380 659 404">C₈H₁₄O₂</p> <p data-bbox="243 500 464 524">CAS # 27829-72-7</p> <p data-bbox="243 623 541 647">Log K_{ow}: 2.61 (EPI Suite)</p> <p data-bbox="243 683 548 708">Molecular Weight: 142.19</p> <p data-bbox="243 743 898 768">Vapor Pressure: 0.881 mm Hg @ 20°C (EPI Suite v4.0)</p> <p data-bbox="243 803 716 828">Water Solubility: 480.5 mg/L (EPI Suite)</p>	<p data-bbox="1058 472 1430 496">-Hexenoic acid, ethyl ester, (E)-</p> <p data-bbox="1115 532 1373 557">Ethyl (E)-2-hexenoate</p> <p data-bbox="1052 592 1442 617">Ethyl <i>trans</i>-2-hexenoate Principal</p> <p data-bbox="1129 652 1358 677">Ethyl hex-2-enoate</p>	 <p>The structure shows a six-carbon chain with a double bond between carbons 2 and 3 in a trans configuration. A carboxylate group is attached to carbon 1, and an ethyl group is attached to the oxygen of the ester linkage. The methyl group at the end of the chain is labeled H₃C.</p>
<p data-bbox="373 872 831 896">Ethyl 3-hydroxy-3-phenylpropionate</p> <p data-bbox="548 930 659 954">C₁₁H₁₄O₃</p> <p data-bbox="243 1053 453 1078">CAS # 5764-85-2</p> <p data-bbox="243 1177 541 1201">Log K_{ow}: 1.52 (EPI Suite)</p> <p data-bbox="243 1237 548 1261">Molecular Weight: 194.23</p> <p data-bbox="243 1297 957 1321">Vapor Pressure: 0.0000381 mm Hg @ 20°C (EPI Suite v4.0)</p> <p data-bbox="243 1357 709 1382">Water Solubility: 7553 mg/L (EPI Suite)</p>	<p data-bbox="999 992 1493 1078">Benzenepropanoic acid, β-hydroxy-, ethyl ester</p> <p data-bbox="1031 1114 1461 1138">Ethyl 3-hydroxy-3-phenylpropanoate</p> <p data-bbox="1037 1174 1455 1198">Ethyl 3-hydroxy-3-phenylpropionate</p> <p data-bbox="1089 1234 1402 1258">Ethyl 3-phenylhydracrylate</p>	 <p>The structure shows a three-carbon chain. Carbon 1 is part of an ethyl ester group. Carbon 2 has a hydroxyl group (OH) attached. Carbon 3 is attached to a phenyl ring. The methyl group at the end of the ethyl group is labeled H₃C.</p>

Table 1: Material Identification		
Material	Synonyms	Structure
<p>Ethyl 2-methyl-2-butenolate*</p> <p>C₇H₁₂O₂</p> <p>CAS # 55514-48-2</p> <p>Log K_{ow}: 2.18 (EPI Suite)</p> <p>Molecular Weight: 128.17</p> <p>Vapor Pressure: 2.17 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1289 mg/L (EPI Suite)</p> <p>*Additional Material for Main CAS # 5837-78-5</p>	<p>2-Butenoic acid, 2-methyl-, ethyl ester</p> <p>Ethyl 2-methyl-2-butenolate</p> <p>Ethyl 2-methylbut-2-enoate</p>	

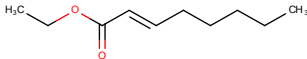
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Ethyl oct-2-enoate</p> <p>C₁₀H₁₈O₂</p> <p>CAS # 2351-90-8</p> <p>Log K_{ow}: 3.6 (EPI Suite)</p> <p>Molecular Weight: 170.25</p> <p>Vapor Pressure: 0.103 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 52.1 mg/L (EPI Suite)</p>	<p>2-Octenoic acid, ethyl ester</p> <p>Ethyl oct-2-enoate</p>	 <p>The chemical structure shows an ethyl group (H₃C-CH₂-) attached to an oxygen atom, which is part of an ester linkage to a carbonyl group (C=O). This carbonyl carbon is also bonded to a double bond (C=C) at the 2-position of an 8-carbon chain. The chain ends with a methyl group (CH₃).</p>

Table 1: Material Identification

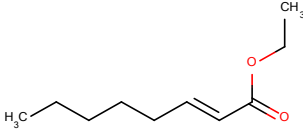
Material	Synonyms	Structure
<p data-bbox="449 321 758 345">Ethyl <i>trans</i>-2-octenoate*</p> <p data-bbox="552 380 655 404">C₁₀H₁₈O₂</p> <p data-bbox="243 500 453 524">CAS # 7367-82-0</p> <p data-bbox="243 623 527 647">Log K_{ow}: 3.6 (EPI Suite)</p> <p data-bbox="243 683 548 708">Molecular Weight: 170.25</p> <p data-bbox="243 743 842 768">Vapor Pressure: 0.156 mm Hg @ 25°C (EPI Suite)</p> <p data-bbox="243 803 699 828">Water Solubility: 52.1 mg/L (EPI Suite)</p> <p data-bbox="243 927 789 951">*Additional Material for Main CAS # 2351-90-8</p>	<p data-bbox="1083 500 1409 524">2-Octenoic acid, ethyl ester</p> <p data-bbox="1010 560 1482 584">Ethyl oct-2-enoate2-Octenoic acid, ethyl</p> <p data-bbox="1184 620 1304 644">ester, (E)-</p> <p data-bbox="1108 680 1381 704">Ethyl <i>trans</i>-2-octenoate</p> <p data-bbox="1136 740 1354 764">Ethyl oct-2-enoate</p>	 <p>The chemical structure shows a trans-2-octenoate ester. It consists of an eight-carbon chain with a double bond between the second and third carbons in a trans configuration. The first carbon is part of an ethyl ester group (-COOCH₂CH₃), with the carbonyl oxygen and the ethyl group's oxygen highlighted in red. The eighth carbon is a methyl group (H₃C).</p>

Table 1: Material Identification

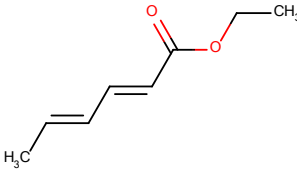
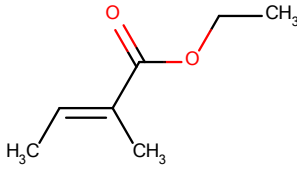
Material	Synonyms	Structure
<p>Ethyl sorbate</p> <p>C₈H₁₂O₂</p> <p>CAS # 2396-84-1</p> <p>Log K_{ow}: 2.4 (EPI Suite)</p> <p>Molecular Weight: 140.18</p> <p>Vapor Pressure: 0.307 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 747.7 mg/L (EPI Suite)</p>	<p>2,4-Hexadienoic acid, ethyl ester, (E,E)-</p> <p>Ethyl 2,4-hexadienoate</p> <p>Ethyl hexa-2,4-dienoate</p> <p>Ethyl sorbate</p>	 <p>The structure shows a six-carbon chain with two conjugated double bonds in the (E,E) configuration. The first double bond is between carbons 2 and 3, with a methyl group (H₃C) attached to carbon 2. The second double bond is between carbons 4 and 5. Carbon 6 is part of an ethyl ester group (-COOCH₂CH₃).</p>
<p>Ethyl tiglate</p> <p>C₇H₁₂O₂</p> <p>CAS # 5837-78-5</p> <p>Log K_{ow}: 2.18 (EPI Suite)</p> <p>Molecular Weight: 128.17</p> <p>Vapor Pressure: 2.17 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1289 mg/L (EPI Suite)</p>	<p>2-Butenoic acid, 2-methyl-, ethyl ester, (E)</p> <p>Ethyl (E)-2-methyl-2-butenate</p> <p>Ethyl α-methylcrotonate</p> <p>Ethyl trans-2-methylcrotonate</p> <p>Ethyl 2-methylbut-2-enoate</p> <p>Ethyl 2-methylcrotonate</p> <p>Ethyl tiglate</p>	 <p>The structure shows a four-carbon chain with a double bond between carbons 2 and 3 in the (E) configuration. Carbon 2 has a methyl group (CH₃) attached. Carbon 3 is part of an ethyl ester group (-COOCH₂CH₃).</p>

Table 1: Material Identification

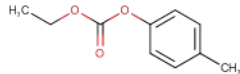
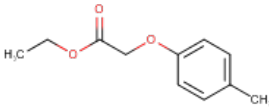
Material	Synonyms	Structure
<p>Ethyl <i>p</i>-tolyl carbonate</p> <p>C₁₀H₁₂O₃</p> <p>CAS # 22719-81-9</p> <p>Log K_{ow}: 2.49 (EPI Suite)</p> <p>Molecular Weight: 180.20</p> <p>Vapor Pressure: 0.00713 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 411.6 mg/L (EPI Suite)</p>	<p>Carbonic acid, ethyl 4-methylphenyl ester</p> <p>Ethyl <i>p</i>-tolyl carbonate</p> <p>Ethyl 4-methylphenyl carbonate</p>	 <chem>CCOC(=O)Oc1ccc(C)cc1</chem>
<p>Ethyl (<i>p</i>-tolylloxy)acetate</p> <p>C₁₁H₁₄O₃</p> <p>CAS # 67028-40-4</p> <p>Log K_{ow}: 2.65 (EPI Suite)</p> <p>Molecular Weight: 194.23</p> <p>Vapor Pressure: 0.00361 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 253.9 mg/L (EPI Suite)</p>	<p>Acetic acid, (4-methylphenoxy)-, ethyl ester</p> <p>Ethyl (<i>p</i>-tolylloxy)acetate</p> <p>Ethyl (4-methylphenoxy)acetate</p> <p>Ethyl <i>p</i>-cresoxyacetate</p>	 <chem>CCOC(=O)COc1ccc(C)cc1</chem>

Table 1: Material Identification

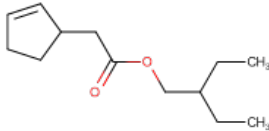
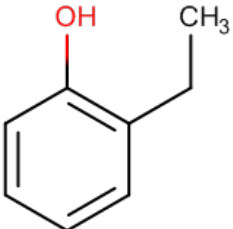
Material	Synonyms	Structure
<p>2-Ethylbutyl cyclopent-2-ene-1-acetate</p> <p>$C_{13}H_{22}O_2$</p> <p>CAS # 94278-39-4</p> <p>Log K_{ow}: 4.81 (EPI Suite)</p> <p>Molecular Weight: 210.31</p> <p>Vapor Pressure: 0.00843 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 3.022 mg/L (EPI Suite)</p>	<p>2-Cyclopentene-1-acetic acid, 2-ethylbutyl ester</p> <p>2-Ethylbutyl cyclopent-2-ene-1-acetate</p>	 <p>The structure shows a cyclopentene ring with an acetate group (-COO-) attached to the 1-position. The ester oxygen is connected to a 2-ethylbutyl chain, which consists of a four-carbon chain with an ethyl group (-CH2CH3) attached to the second carbon.</p>
<p>2-Ethylphenol</p> <p>$C_8H_{10}O$</p> <p>CAS # 90-00-6</p> <p>Log K_{ow}: 2.55 (EPI Suite)</p> <p>Molecular Weight: 122.16</p> <p>Vapor Pressure: 0.0961 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 2912 mg/L (EPI Suite)</p>	<p>2-Ethylphenol</p> <p>Phenol, 2-ethyl-Phloro</p>	 <p>The structure shows a benzene ring with a hydroxyl group (-OH) at the 1-position and an ethyl group (-CH2CH3) at the 2-position.</p>

Table 1: Material Identification

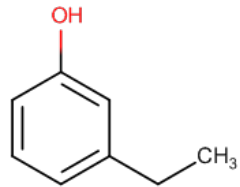
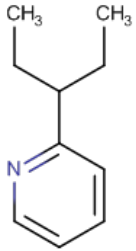
Material	Synonyms	Structure
<p>3-Ethylphenol</p> <p>C₈H₁₀O</p> <p>CAS # 620-17-7</p> <p>Log K_{ow}: 2.55 (EPI Suite)</p> <p>Molecular Weight: 122.16</p> <p>Vapor Pressure: 0.0438 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 3342 mg/L (EPI Suite)</p>	<p><i>m</i>-Ethylphenol</p> <p>3-Ethylphenol</p> <p>Phenol, 3-ethyl</p>	
<p>2-(1-Ethylpropyl)pyridine</p> <p>C₁₀H₁₅N</p> <p>CAS # 7399-50-0</p> <p>Log K_{ow}: 3.24 (EPI Suite)</p> <p>Molecular Weight: 149.23</p> <p>Vapor Pressure: 0.309 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 2595 mg/L (EPI Suite)</p>	<p>2-(1-Ethylpropyl)pyridine</p> <p>2-(3-Pentyl)pyridine</p> <p>Pyridine, 2-(1-ethylpropyl)-</p> <p>Verdima</p>	

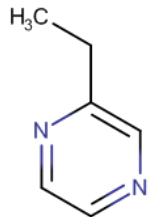
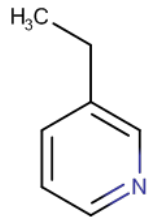
Table 1: Material Identification		
Material	Synonyms	Structure
<p>2-Ethylpyrazine</p> <p>C₆H₈N₂</p> <p>CAS # 13925-00-3</p> <p>Log K_{ow}: 0.98 (EPI Suite)</p> <p>Molecular Weight: 108.14</p> <p>Vapor Pressure: 2.57 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 28410 mg/L (EPI Suite)</p>	<p>2-Ethyl-1,4-diazine</p> <p>2-Ethylpyrazine</p> <p>Pyrazine, ethyl-</p>	
<p>3-Ethylpyridine</p> <p>C₇H₉N</p> <p>CAS # 536-78-7</p> <p>Log K_{ow}: 1.84 (EPI Suite)</p> <p>Molecular Weight: 107.15</p> <p>Vapor Pressure: 1.4 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 84780 mg/L (EPI Suite)</p>	<p>β-Ethylpyridine</p> <p>β-Lutidine</p> <p>3-Ethylpyridine</p> <p>Pyridine, 3-ethyl-</p>	

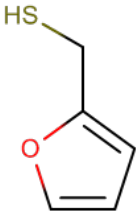
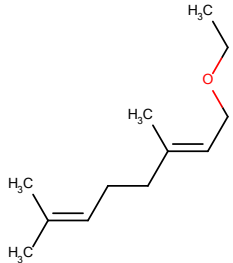
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Furfuryl mercaptan</p> <p>C₅H₆OS</p> <p>CAS # 98-02-2</p> <p>Log K_{ow}: 1.96 (EPI Suite)</p> <p>Molecular Weight: 114.17</p> <p>Vapor Pressure: 2.07 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 2216 mg/L (EPI Suite)</p>	<p>α-Furfuryl mercaptan</p> <p>2-Furanmethanethiol</p> <p>2-Furylmethanethiol</p> <p>Furfuryl mercaptan</p>	
<p>Geranyl ethyl ether</p> <p>C₁₂H₂₂O</p> <p>CAS # 40267-72-9</p> <p>Log K_{ow}: 4.66 (EPI Suite)</p> <p>Molecular Weight: 182.30</p> <p>Vapor Pressure: 0.0934 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 5.618 mg/L (EPI Suite)</p>	<p>1-Ethoxy-3,7-dimethyl-2,6-octadiene</p> <p>1-Ethoxy-3,7-dimethylocta-2,6-diene</p> <p>2,6-Octadiene, 1-ethoxy-3,7-dimethyl-</p> <p>2,6-ジメチル-8-エトキシ-2,6-オクタジエン</p> <p>Ethyl geranyl ether</p> <p>Geranyl ethyl ether</p>	

Table 1: Material Identification

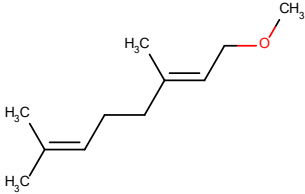
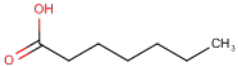
Material	Synonyms	Structure
<p>Geranyl methyl ether</p> <p>C₁₁H₂₀O</p> <p>CAS # 2565-82-4</p> <p>Log K_{ow}: 4.17 (EPI Suite)</p> <p>Molecular Weight: 168.28</p> <p>Vapor Pressure: 0.243 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 17.23 mg/L (EPI Suite)</p>	<p>(E)-1-Methoxy-3,7-dimethylocta-2,6-dien</p> <p>1-Methoxy-3,7-dimethylocta-2,6-diene</p> <p>2,6-Octadiene, 1-methoxy-3,7-dimethyl-,</p> <p>(E)-</p> <p>Geranyl methyl ether</p>	 <p>The structure shows a zigzag carbon chain with two double bonds. The first double bond is at the 2-position and has two methyl groups (H₃C) attached. The second double bond is at the 6-position and has a methyl group (H₃C) and a methoxy group (-OCH₃) attached. The methoxy group is shown in red.</p>
<p>Heptanoic acid</p> <p>C₇H₁₄O₂</p> <p>CAS # 111-14-8</p> <p>Log K_{ow}: 2.45 (EPI Suite)</p> <p>Molecular Weight: 130.18</p> <p>Vapor Pressure: 0.0769 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1955 mg/L (EPI Suite)</p>	<p><i>n</i>-Heptylic acid</p> <p>Enanthic acid</p> <p>Heptanoic acid</p> <p>Oenanthic acid</p> <p>Oenanthylic acid</p> <p>アルカン酸(C=4~30)</p>	 <p>The structure shows a zigzag carbon chain with a carboxylic acid group (-COOH) at one end. The carboxyl group is shown in red.</p>

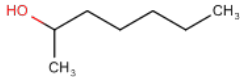
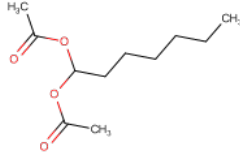
Table 1: Material Identification		
Material	Synonyms	Structure
<p>2-Heptanol</p> <p>C₇H₁₆O</p> <p>CAS # 543-49-7</p> <p>Log K_{ow}: 2.24 (EPI Suite)</p> <p>Molecular Weight: 116.20</p> <p>Vapor Pressure: 0.574 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 3569 mg/L (EPI Suite)</p>	<p>sec-Heptyl alcohol</p> <p>2-Heptanol</p> <p>2-Hydroxyheptane</p> <p>Amyl methyl carbinol</p> <p>Heptan-2-ol</p>	
<p>Heptylidene diacetate</p> <p>C₁₁H₂₀O₄</p> <p>CAS # 56438-09-6</p> <p>Log K_{ow}: 2.79 (EPI Suite)</p> <p>Molecular Weight: 216.27</p> <p>Vapor Pressure: 0.0422 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 150.2 mg/L (EPI Suite)</p>	<p>1,1-Heptanediol, diacetate</p> <p>Heptane-1,1-diyl diacetate</p> <p>Heptylidene diacetate</p>	

Table 1: Material Identification

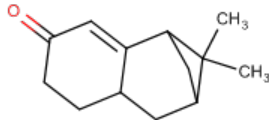
Material	Synonyms	Structure
<p data-bbox="348 321 856 407">2,3,4,4a,5,6-hexahydro-2,2-dimethyl-1,3-methanonaphthalen-7(1H)-one</p> <p data-bbox="552 440 653 467">C₁₃H₁₈O</p> <p data-bbox="243 561 468 589">CAS # 68433-81-8</p> <p data-bbox="243 683 541 711">Log K_{ow}: 3.11 (EPI Suite)</p> <p data-bbox="243 743 548 771">Molecular Weight: 190.28</p> <p data-bbox="243 803 930 831">Vapor Pressure: 0.00312 mm Hg @ 20°C (EPI Suite v4.0)</p> <p data-bbox="243 863 695 891">Water Solubility: 108 mg/L (EPI Suite)</p>	<p data-bbox="1003 472 1486 683">1,3-Methanonaphthalen-7(1H)-one, 2,3,4,4a,5,6-hexahydro-2,2-dimethyl-, 2,3,4,4a,5,6-hexahydro-2,2-dimethyl-1,3- methanonaphthalen-7(1H)-one</p> <p data-bbox="1182 716 1308 743">Tricyclone</p>	 <p>The chemical structure of Tricyclone is a tricyclic system consisting of a six-membered ring fused to a five-membered ring, which is further fused to a four-membered ring. A carbonyl group (C=O) is attached to the six-membered ring. Two methyl groups (CH₃) are attached to the four-membered ring.</p>

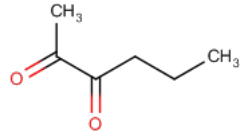
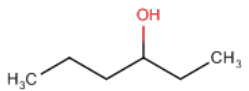
Table 1: Material Identification		
Material	Synonyms	Structure
<p>2,3-Hexanedione</p> <p>$C_6H_{10}O_2$</p> <p>CAS # 3848-24-6</p> <p>Log K_{ow}: -0.35 (EPI Suite)</p> <p>Molecular Weight: 114.14</p> <p>Vapor Pressure: 2.11 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 211300 mg/L (EPI Suite)</p>	<p>2,3-Hexanedione</p> <p>Acetylbutyryl</p> <p>Butyryl acetyl</p> <p>Hexane-2,3-dione</p> <p>Methyl propyl diketone</p>	
<p>3-Hexanol</p> <p>$C_6H_{14}O$</p> <p>CAS # 623-37-0</p> <p>Log K_{ow}: 1.75 (EPI Suite)</p> <p>Molecular Weight: 102.17</p> <p>Vapor Pressure: 2.17 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 14530 mg/L (EPI Suite)</p>	<p>3-Hexanol</p> <p>Carbinol EP</p> <p>Ethyl propyl carbinol</p> <p>Hexan-3-ol</p>	

Table 1: Material Identification

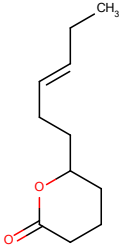
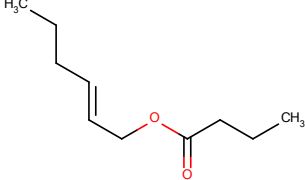
Material	Synonyms	Structure
<p>6-(3Z)-3-Hexen-1-yltetrahydro-2H-pyran-2-one,</p> <p>C₁₁H₁₈O₂</p> <p>CAS # 68959-28-4</p> <p>Log K_{ow}: 2.84 (EPI Suite)</p> <p>Molecular Weight: 182.26</p> <p>Vapor Pressure: 0.00086 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 200.3 mg/L (EPI Suite)</p>	<p>(Z)-6-(3-Hexenyl)tetrahydro-2H-pyran-2-one</p> <p>2H-Pyran-2-one, 6-(3-hexenyl)tetrahydro-,</p> <p>(Z)-</p> <p>5-Hydroxy-8-undecenoic acid delta-lactone</p> <p>6-(3Z)-3-hexen-1-yltetrahydro-2H-Pyran-2-one,</p> <p>Jasmolactone extra C</p>	
<p>trans-2-Hexenyl butyrate</p> <p>C₁₀H₁₈O₂</p> <p>CAS # 53398-83-7</p> <p>Log K_{ow}: 3.6 (EPI Suite)</p> <p>Molecular Weight: 170.25</p> <p>Vapor Pressure: 0.103 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 52.1 mg/L (EPI Suite)</p>	<p>(E)-2-Hexenyl butyrate</p> <p>(E)-Hex-2-enyl butyrate</p> <p>trans-2-Hexenyl butanoate</p> <p>trans-2-Hexenyl butyrate</p> <p>Butanoic acid, 2-hexenyl ester, (E)</p> <p>Hex-2-en-1-yl butyrate</p> <p>アルカ酸(C=1~6)アルケニル(C=4~8)</p>	

Table 1: Material Identification

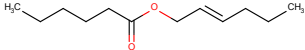
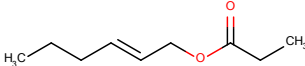
Material	Synonyms	Structure
<p><i>trans</i>-2-Hexenyl hexanoate</p> <p>C₁₂H₂₂O₂</p> <p>CAS # 53398-86-0</p> <p>Log K_{ow}: 4.58 (EPI Suite)</p> <p>Molecular Weight: 198.30</p> <p>Vapor Pressure: 0.0145 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 5.496 mg/L (EPI Suite)</p>	<p>(E)Hex-2-enyl hexanoate</p> <p><i>trans</i>-2-Hexenyl caproate</p> <p><i>trans</i>-2-Hexenyl hexanoate</p> <p>Hex-2-en-1-yl hexanoate</p> <p>Hexanoic acid, (2E)-2-hexenyl ester</p> <p>アルカン酸(C=1~6)アルケニル(C=4~8)</p>	 <p>The structure shows a hexanoate chain (left) connected via an ester oxygen to a trans-2-hexenyl chain (right). The ester oxygen is highlighted in red. The trans configuration is shown with the two alkyl chains on the double bond on opposite sides.</p>
<p><i>trans</i>-2-Hexenyl propionate</p> <p>C₉H₁₆O₂</p> <p>CAS # 53398-80-4</p> <p>Log K_{ow}: 3.1 (EPI Suite)</p> <p>Molecular Weight: 156.22</p> <p>Vapor Pressure: 0.284 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 158.9 mg/L (EPI Suite)</p>	<p>(E)-2-Hexenyl propionate</p> <p>(E)-Hex-2-enyl propionate</p> <p><i>trans</i>-2-Hexenyl propionate</p> <p>2-Hexen-1-ol, propanoate, (E)-</p> <p>Hex-2-en-1-yl propionate</p>	 <p>The structure shows a propionate chain (left) connected via an ester oxygen to a trans-2-hexenyl chain (right). The ester oxygen is highlighted in red. The trans configuration is shown with the two alkyl chains on the double bond on opposite sides.</p>

Table 1: Material Identification

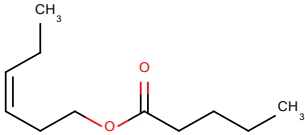
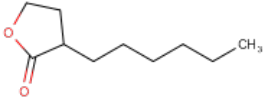
Material	Synonyms	Structure
<p><i>cis</i>-3-Hexenyl valerate</p> <p>C₁₁H₂₀O₂</p> <p>CAS # 35852-46-1</p> <p>Log K_{ow}: 4.09 (EPI Suite)</p> <p>Molecular Weight: 184.27</p> <p>Vapor Pressure: 0.0382 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 16.97 mg/L (EPI Suite)</p>	<p>Z)-3-Hexenyl valerate</p> <p>(Z)-Hex-3-enyl valerate</p> <p><i>cis</i>-3-Hexenyl pentanoate</p> <p><i>cis</i>-3-Hexenyl valerate I</p> <p>Hex-3-en-1-yl valerate</p> <p>Pentanoic acid, 3-hexenyl ester, (Z)-</p> <p>Valeric acid, 3-hexenyl ester, (z</p>	 <p>The structure shows a valeric acid chain (5 carbons) with a methyl group at the end, esterified to a 3-hexenyl chain. The double bond in the 3-hexenyl chain is in the cis configuration. The ester oxygen is highlighted in red.</p>
<p>3-Hexyldihydrofuran-2(3H)-one</p> <p>C₁₀H₁₈O₂</p> <p>CAS # 18436-37-8</p> <p>Log K_{ow}: 2.57 (EPI Suite)</p> <p>Molecular Weight: 170.25</p> <p>Vapor Pressure: 00.00317 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 393.8 mg/L (EPI Suite)</p>	<p>α-Hexyl-γ-butyrolactone</p> <p>2(3H)-Furanone, 3-hexyldihydro-</p> <p>3-Hexyldihydrofuran-2(3H)-one</p> <p>Octanoic acid, 2-(2-hydroxyethyl)-, γ-lactone</p>	 <p>The structure shows a five-membered lactone ring (gamma-butyrolactone) with a 3-hexyl group attached to the 2-position. The ring oxygen is highlighted in red.</p>

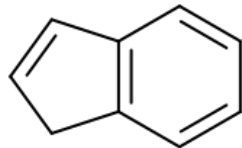
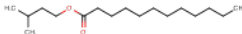
Table 1: Material Identification		
Material	Synonyms	Structure
<p>1H-Indene</p> <p>C₉H₈</p> <p>CAS # 95-13-6</p> <p>Log K_{ow}: 3.25 (EPI Suite)</p> <p>Molecular Weight: 116.16</p> <p>Vapor Pressure: 0.607 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 332.4 mg/L (EPI Suite)</p>	<p>1H-Indene</p> <p>Indene</p> <p>Indonaphthene</p>	
<p>Isoamyl laurate</p> <p>C₁₇H₃₄O₂</p> <p>CAS # 6309-51-9</p> <p>Log K_{ow}: 7.17 (EPI Suite)</p> <p>Molecular Weight: 270.45</p> <p>Vapor Pressure: 0.00054 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 0.01354 mg/L (EPI Suite)</p>	<p>3-Methylbutyl laurate</p> <p>Amyl(iso) laurate</p> <p>Dodecanoic acid, 3-methylbutyl ester</p> <p>Isoamyl dodecanoate</p> <p>Isoamyl laurate Principal</p> <p>Isopentyl dodecanoate</p> <p>Isopentyl dodecylate</p> <p>Isopentyl laurate</p>	

Table 1: Material Identification

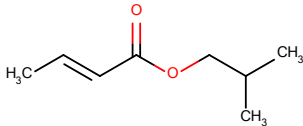
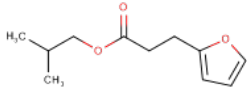
Material	Synonyms	Structure
<p>Isobutyl 2-butenate</p> <p>C₈H₁₄O₂</p> <p>CAS # 589-66-2</p> <p>Log K_{ow}: 2.54 (EPI Suite)</p> <p>Molecular Weight: 142.19</p> <p>Vapor Pressure: 1.49 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 555.2 mg/L (EPI Suite)</p>	<p>2-Butenoic acid, 2-methylpropyl ester</p> <p>2-Methylpropyl 2-butenate</p> <p>Isobutyl 2-butenate</p> <p>Isobutyl but-2-enoate</p> <p>Isobutyl crotonate</p>	 <p>The structure shows a 2-butenate group (H₃C-CH=CH-C(=O)-O-) attached to an isobutyl group (-CH₂-CH(CH₃)₂).</p>
<p>Isobutyl 3-(2-furan)propionate</p> <p>C₁₁H₁₆O₃</p> <p>CAS # 105-01-1</p> <p>Log K_{ow}: 3.34 (EPI Suite)</p> <p>Molecular Weight: 196.24</p> <p>Vapor Pressure: 0.0181 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 64.04 mg/L (EPI Suite)</p>	<p>2-Furanpropionic acid, 2-methylpropyl ester</p> <p>Isobutyl 2-furanpropionate</p> <p>Isobutyl 2-furylpropionate</p> <p>Isobutyl 3-(2-furan)propionate</p> <p>Isobutyl 3-(2-furyl)propanoate</p> <p>Isobutyl furylpropionate</p>	 <p>The structure shows a 3-(2-furan)propionate group (-CH₂-CH₂-C(=O)-O-) attached to an isobutyl group (-CH₂-CH(CH₃)₂).</p>

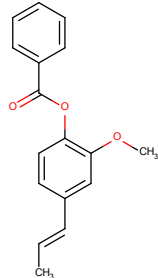
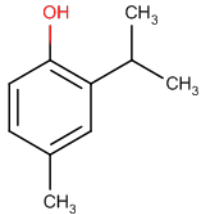
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Isoeugenol benzoate</p> <p>$C_{17}H_{16}O_3$</p> <p>CAS # 4194-00-7</p> <p>Log K_{ow}: 4.44 (EPI Suite)</p> <p>Molecular Weight: 268.31</p> <p>Vapor Pressure: 0.00000252 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 3.015 mg/L (EPI Suite)</p>	<p>2-Methoxy-4-prop-1-en-1-ylphenyl benzoate</p> <p>2-Methoxy-4-prop-1-enylphenyl benzoate</p> <p>Isoeugenol benzoate</p> <p>Isoeugenyl benzoate</p> <p>Phenol, 2-methoxy-4-(1-propenyl)-, benzoate</p>	
<p>2-Isopropyl-<i>p</i>-cresol</p> <p>$C_{10}H_{14}O$</p> <p>CAS # 4427-56-9</p> <p>Log K_{ow}: 3.52 (EPI Suite)</p> <p>Molecular Weight: 150.22</p> <p>Vapor Pressure: 0.0163 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 286 mg/L (EPI Suite)</p>	<p><i>m</i>-Cymen-4-ol</p> <p>2-Isopropyl-<i>p</i>-cresol</p> <p>2-Isopropyl-4-methylphenol</p> <p>4-Methyl-2-(1-methylethyl)phenol</p> <p>Galbanum Phenol</p> <p>Isothymol</p> <p>Phenol, 4-methyl-2-(1-methylethyl)-</p>	

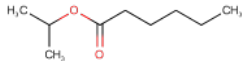
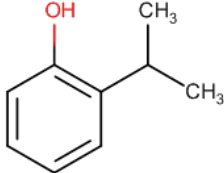
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Isopropyl hexanoate</p> <p>C₉H₁₈O₂</p> <p>CAS # 2311-46-8</p> <p>Log K_{ow}: 3.25 (EPI Suite)</p> <p>Molecular Weight: 158.24</p> <p>Vapor Pressure: 0.726 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 117.8 mg/L (EPI Suite)</p>	<p>Hexanoic acid, 1-methylethyl ester</p> <p>Isopropyl caproate</p> <p>Isopropyl capronate</p> <p>Isopropyl hexanoate</p> <p>Isopropyl hexylate</p> <p>アルカン酸(C=6~10)アルキル(C=1~10)</p>	
<p>2-Isopropylphenol</p> <p>C₉H₁₂O</p> <p>CAS # 88-69-7</p> <p>Log K_{ow}: 2.97 (EPI Suite)</p> <p>Molecular Weight: 136.19</p> <p>Vapor Pressure: 0.0579 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1146 mg/L (EPI Suite)</p>	<p>o-Cumenol</p> <p>o-Isopropylphenol</p> <p>1-Hydroxy-2-isopropylbenzene</p> <p>2-Isopropylphenol</p> <p>Phenol, 2-(1-methylethyl)-</p>	

Table 1: Material Identification

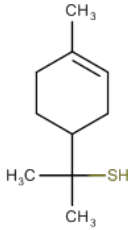
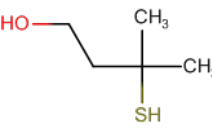
Material	Synonyms	Structure
<p>1-<i>p</i>-Menthene-8-thiol</p> <p>C₁₀H₁₈S</p> <p>CAS # 71159-90-5</p> <p>Log K_{ow}: 4.74 (EPI Suite)</p> <p>Molecular Weight: 170.31</p> <p>Vapor Pressure: 0.0695 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 5.485 mg/L (EPI Suite)</p>	<p>α,α,4-Trimethyl-3-cyclohexen-1-methanethiol</p> <p>1-<i>p</i>-Menthene-8-thiol</p> <p>3-Cyclohexene-1-methanethiol, α,α,4-trimethyl-</p>	
<p>3-Mercapto-3-methyl-1-butanol</p> <p>C₅H₁₂OS</p> <p>CAS # 34300-94-2</p> <p>Log K_{ow}: 1.16 (EPI Suite)</p> <p>Molecular Weight: 120.21</p> <p>Vapor Pressure: 0.135 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 10100 mg/L (EPI Suite)</p>	<p>1-Butanol, 3-mercapto-3-methyl-</p> <p>3-Mercapto 3-Methyl Butanol</p> <p>3-Mercapto-3-methyl-1-butanol</p> <p>3-Mercapto-3-methylbutyl alcohol</p> <p>3-Methyl-3-mercaptobutyl alcohol</p>	

Table 1: Material Identification

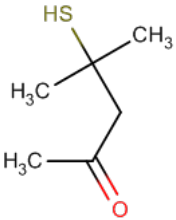
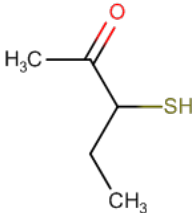
Material	Synonyms	Structure
<p>4-Mercapto-4-methyl-2-pentanone</p> <p>C₆H₁₂OS</p> <p>CAS # 19872-52-7</p> <p>Log K_{ow}: 1.07 (EPI Suite)</p> <p>Molecular Weight: 132.22</p> <p>Vapor Pressure: 0.924 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 10970 mg/L (EPI Suite)</p>	<p>2-Mercapto-2-methyl-4-pentanone</p> <p>2-Mercapto-2-methylpentan-4-one</p> <p>2-methyl-4-oxopentane-2-thiol</p> <p>2-Pentanone, 4-mercapto-4-methyl-</p> <p>4-Mercapto-4-methyl-2-pentanone</p> <p>4-Mercapto-4-methylpentan-2-one</p> <p>4-Methyl-4-mercapto-2-pentanone</p> <p>4-Methyl-4-sulfanylpentan-2-one</p> <p>Thiomethyl pentanone-4,4,2</p>	 <p>The structure shows a five-carbon chain. The second carbon from the right has a double bond to an oxygen atom (red) and a methyl group (H₃C). The fourth carbon from the right has a methyl group (CH₃) and a thiol group (HS) attached to it.</p>
<p>3-Mercapto-2-pentanone</p> <p>C₅H₁₀OS</p> <p>CAS # 67633-97-0</p> <p>Log K_{ow}: 0.62 (EPI Suite)</p> <p>Molecular Weight: 118.19</p> <p>Vapor Pressure: 2.44 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 30260 mg/L (EPI Suite)</p>	<p>2-Pentanone, 3-mercapto-</p> <p>3-Mercapto-2-pentanone</p> <p>3-Sulfanylpentan-2-one</p> <p>Carthione-013</p>	 <p>The structure shows a five-carbon chain. The second carbon from the right has a double bond to an oxygen atom (red) and a methyl group (H₃C). The third carbon from the right has a thiol group (SH) attached to it.</p>

Table 1: Material Identification

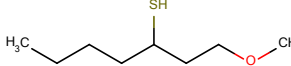
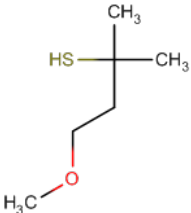
Material	Synonyms	Structure
<p data-bbox="422 321 779 347">(S1)-Methoxy-3-heptanethiol</p> <p data-bbox="548 380 653 406">C₈H₁₈OS</p> <p data-bbox="243 500 485 526">CAS # 400052-49-5</p> <p data-bbox="243 623 541 649">Log K_{ow}: 2.88 (EPI Suite)</p> <p data-bbox="243 682 548 708">Molecular Weight: 162.29</p> <p data-bbox="243 740 842 766">Vapor Pressure: 0.299 mm Hg @ 25°C (EPI Suite)</p> <p data-bbox="243 799 716 824">Water Solubility: 230.2 mg/L (EPI Suite)</p>	<p data-bbox="1073 500 1409 526">(S1)-Methoxy-3-heptanethiol</p> <p data-bbox="1052 558 1430 584">3-Heptanethiol, 1-methoxy-, (3S)</p> <p data-bbox="1178 617 1304 643">ARUSCOL</p>	 <p>The structure shows a seven-carbon chain. The third carbon from the left has a thiol group (-SH) attached. The first carbon from the right has a methoxy group (-OCH₃) attached. The chain is labeled with H₃C at the left end and CH₃ at the right end.</p>
<p data-bbox="390 873 810 899">4-Methoxy-2-methyl-2-butanethiol</p> <p data-bbox="548 932 653 958">C₆H₁₄OS</p> <p data-bbox="243 1052 464 1078">CAS # 94087-83-9</p> <p data-bbox="243 1175 541 1201">Log K_{ow}: 1.86 (EPI Suite)</p> <p data-bbox="243 1234 548 1260">Molecular Weight: 134.24</p> <p data-bbox="243 1292 873 1318">Vapor Pressure: 2.4 mm Hg @ 20°C (EPI Suite v4.0)</p> <p data-bbox="369 1351 831 1377">Water Solubility: 2263 mg/L (EPI Suite)</p>	<p data-bbox="1041 1084 1451 1110">2-Butanethiol, 4-methoxy-2-methyl-</p> <p data-bbox="1041 1143 1440 1169">4-Methoxy-2-methyl-2-butanethiol</p>	 <p>The structure shows a four-carbon chain. The second carbon from the left has a thiol group (-SH) and a methyl group (-CH₃) attached. The fourth carbon from the left has a methoxy group (-OCH₃) attached. The chain is labeled with H₃C at the left end and CH₃ at the right end.</p>

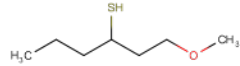
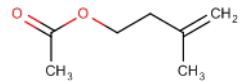
Table 1: Material Identification		
Material	Synonyms	Structure
<p>1-Methoxyhexane-3-thiol</p> <p>C₇H₁₆OS</p> <p>CAS # 94291-50-6</p> <p>Log K_{ow}: 2.3 (EPI Suite)</p> <p>Molecular Weight: 148.26</p> <p>Vapor Pressure: 0.561 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 698.7 mg/L (EPI Suite)</p>	<p>1-Methoxyhexane-3-thiol</p> <p>3-Hexanethiol, 1-methoxy-</p> <p>Sclarymol</p>	
<p>3-Methyl-3-butenyl acetate</p> <p>C₇H₁₂O₂</p> <p>CAS # 5205-07-2</p> <p>Log K_{ow}: 2.26 (EPI Suite)</p> <p>Molecular Weight: 128.17</p> <p>Vapor Pressure: 4.51 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1104 mg/L (EPI Suite)</p>	<p>3-Buten-1-ol, 3-methyl-, acetate</p> <p>3-Methyl-3-butenyl acetate</p> <p>3-Methylbut-3-en-1-yl acetate</p> <p>Isoprenyl acetate</p> <p>アルカン酸(C=1~6)アルケニル(C=4~8)</p>	

Table 1: Material Identification

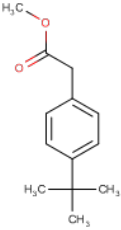
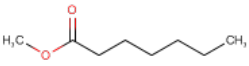
Material	Synonyms	Structure
<p>Methyl <i>p</i>-tert-butylphenylacetate</p> <p>C₁₃H₁₈O₂</p> <p>CAS # 3549-23-3</p> <p>Log K_{ow}: 3.99 (EPI Suite)</p> <p>Molecular Weight: 206.28</p> <p>Vapor Pressure: 0.00363 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 15.88 mg/L (EPI Suite)</p>	<p>Benzeneacetic acid, 4-(1,1-dimethylethyl)-, methyl ester</p> <p>Methyl (4-tert-butylphenyl)acetate</p> <p>Methyl <i>p</i>-tert-butylphenylacetate</p>	 <p>The structure shows a central benzene ring. At the top position, there is a methyl ester group (-COOCH₃). At the bottom position, there is a tert-butyl group (-C(CH₃)₃). The two groups are para to each other.</p>
<p>Methyl heptanoate</p> <p>C₈H₁₆O₂</p> <p>CAS # 106-73-0</p> <p>Log K_{ow}: 2.83 (EPI Suite)</p> <p>Molecular Weight: 144.21</p> <p>Vapor Pressure: 0.904 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 308.7 mg/L (EPI Suite)</p>	<p>Heptanoic acid, methyl ester</p> <p>Methyl heptanoate</p> <p>Methyl heptoate</p> <p>Methyl heptylate</p> <p>Methyl oenanthatate</p> <p>アルカン酸(C=6~10)アルキル(C=1~10)</p>	 <p>The structure shows a methyl ester group (-COOCH₃) on the left, connected to a seven-carbon alkyl chain ending in a methyl group (-CH₃) on the right.</p>

Table 1: Material Identification		
Material	Synonyms	Structure
<p>Methyl-(E)-hex-2-enoate *</p> <p>$C_7H_{12}O_2$</p> <p>CAS # 13894-63-8</p> <p>Log K_{ow}: 2.12 (EPI Suite)</p> <p>Molecular Weight: 128.17</p> <p>Vapor Pressure: 2.26 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1439 mg/L (EPI Suite)</p> <p>*Additional Material for Main CAS # 2396-77-2</p>	<p>2-Hexenoic acid, methyl ester, (E)-</p> <p>Methyl hex-2-enoate</p> <p>Methyl-(E)-hex-2-enoate</p> <p>Methyl-trans-2-Hexenoate</p>	

Table 1: Material Identification

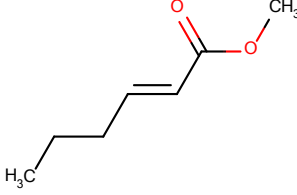
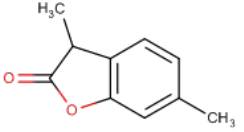
Material	Synonyms	Structure
<p>Methyl 2-hexenoate</p> <p>$C_7H_{12}O_2$</p> <p>CAS # 2396-77-2</p> <p>Log K_{ow}: 2.12 (EPI Suite)</p> <p>Molecular Weight: 128.17</p> <p>Vapor Pressure: 3.15 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 1439 mg/L (EPI Suite)</p>	<p>2-Hexenoic acid, methyl ester</p> <p>Methyl β-propylacrylate</p> <p>Methyl 2-hexenoate</p>	 <p>The structure shows a six-carbon chain with a double bond between the second and third carbons. The second carbon is also part of a methyl ester group (-COOCH3). The terminal carbon is labeled H3C.</p>
<p>2-(4-Methyl-2-hydroxyphenyl)propionic acid-γ-lactone</p> <p>$C_{10}H_{10}O_2$</p> <p>CAS # 65817-24-5</p> <p>Log K_{ow}: 1.44 (EPI Suite)</p> <p>Molecular Weight: 162.18</p> <p>Vapor Pressure: 0.000625 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 3934 mg/L (EPI Suite)</p>	<p>2-(4-Methyl-2-hydroxyphenyl)propionic acid-γ-lactone</p> <p>Dimethyl-3,6-benzo-2(3H)-furanone</p> <p>Furaminton</p>	 <p>The structure shows a benzene ring with a methyl group at the 4-position and a propionic acid-gamma-lactone ring at the 2-position. The methyl group is labeled H3C and the lactone ring has a carbonyl group and an oxygen atom.</p>

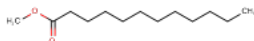
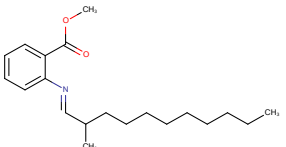
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Methyl laurate</p> <p>$C_{13}H_{26}O_2$</p> <p>CAS # 111-82-0</p> <p>Log K_{ow}: 5.28 (EPI Suite)</p> <p>Molecular Weight: 214.34</p> <p>Vapor Pressure: 0.00671 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 0.8841 mg/L (EPI Suite)</p>	<p>Dodecanoic acid, methyl ester</p> <p>Lauric acid, methyl ester</p> <p>Methyl dodecanoate</p> <p>Methyl dodecylate</p> <p>Methyl laurate</p> <p>脂肪酸(C=9~24)アルキル(C=1~10)エステル</p>	
<p>Methyl 2-[(2-methylundecylidene)amino]benzoate</p> <p>$C_{20}H_{31}NO_2$</p> <p>CAS # 67800-80-0</p> <p>Log K_{ow}: 6.66 (EPI Suite)</p> <p>Molecular Weight: 317.47</p> <p>Vapor Pressure: 0.00000138 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 0.02 mg/L (EPI Suite)</p>	<p>2-Methyldecanal methylanthranilate Schiff base</p> <p>Benzoic acid, 2-[(2-methylundecylidene)amino]-, methyl ester</p> <p>Methyl 2-[(2-methylundecylidene)amino]benzoate</p>	

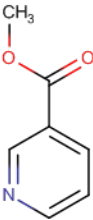
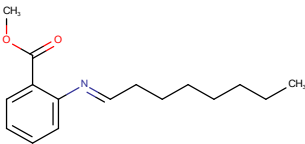
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Methyl nicotinate</p> <p>$C_7H_7NO_2$</p> <p>CAS # 93-60-7</p> <p>Log K_{ow}: 0.64 (EPI Suite)</p> <p>Molecular Weight: 137.13</p> <p>Vapor Pressure: 0.113 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 16830 mg/L (EPI Suite)</p>	<p>3-Carbomethoxypyridine</p> <p>3-Pyridinecarboxylic acid, methyl ester</p> <p>Methyl 3-pyridinecarboxylate</p> <p>Methyl nicotinate</p>	
<p>Methyl 2-(octylideneamino)benzoate</p> <p>$C_{16}H_{23}NO_2$</p> <p>CAS # 67801-44-9</p> <p>Log K_{ow}: 4.77 (EPI Suite)</p> <p>Molecular Weight: 261.36</p> <p>Vapor Pressure: 0.0000242 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1.737 mg/L (EPI Suite)</p>	<p>Artanol DIPG</p> <p>Benzoic acid, 2-(octylideneamino)-, methyl ester</p> <p>Methyl 2-(octylideneamino)benzoate</p> <p>Ocmea</p> <p>Octanal methyl anthranilate Schiff base</p>	

Table 1: Material Identification

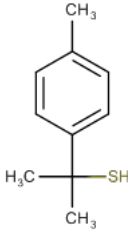
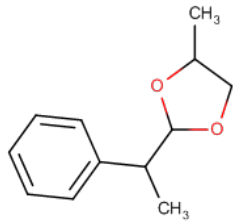
Material	Synonyms	Structure
<p>2-(4-Methyl-1-phenyl)-2-propanethiol</p> <p>C₁₀H₁₄S</p> <p>CAS # 80819-94-9</p> <p>Log K_{ow}: (EPI Suite)</p> <p>Molecular Weight: 166.28</p> <p>Vapor Pressure: 0.051 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 29.76 mg/L (EPI Suite)</p>	<p>2-(4-Methyl-1-phenyl)-2-propanethiol</p>	 <p>The structure shows a central carbon atom bonded to a 4-methylphenyl group (a benzene ring with a methyl group at the para position), two methyl groups, and a thiol (-SH) group.</p>
<p>4-Methyl-2-(1-phenylethyl)-1,3-dioxolane</p> <p>C₁₂H₁₆O₂</p> <p>CAS # 67634-23-5</p> <p>Log K_{ow}: 2.65 (EPI Suite)</p> <p>Molecular Weight: 192.25</p> <p>Vapor Pressure: 0.00606 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 259.6 mg/L (EPI Suite)</p>	<p>1,3-Dioxolane, 4-methyl-2-(1-phenylethyl)-</p> <p>2-Phenylpropanal propyleneglycol acetal</p> <p>4-Methyl-2-(1-phenylethyl)-1,3-dioxolane</p> <p>Cyclotropal</p> <p>Hydrotropic Aldehyde Propylene Glycol</p> <p>Acetal</p>	 <p>The structure shows a 1,3-dioxolane ring with a methyl group at the 4-position and a 1-phenylethyl group at the 2-position.</p>

Table 1: Material Identification

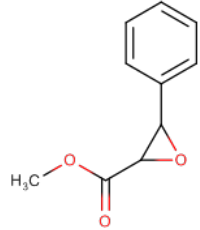
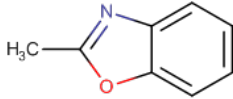
Material	Synonyms	Structure
<p>Methyl β-phenylglycidate</p> <p>C₁₀H₁₀O₃</p> <p>CAS # 37161-74-3</p> <p>Log K_{ow}: 2.06 (EPI Suite)</p> <p>Molecular Weight: 178.18</p> <p>Vapor Pressure: 0.00934 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 985.9 mg/L (EPI Suite)</p>	<p>(+/-)-Methyl 2,3-epoxycinnamate</p> <p>Glycidic acid, 3-phenyl-, methyl ester</p> <p>Methyl β-phenylglycidate</p> <p>Methyl-3-phenyloxirane-2-carboxylate</p>	 <p>The structure shows a benzene ring attached to a three-membered epoxide ring. The epoxide ring is also attached to a carbonyl group (C=O) which is further bonded to a methoxy group (OCH₃).</p>
<p>2-Methylbenzoxazole</p> <p>C₈H₇NO</p> <p>CAS # 95-21-6</p> <p>Log K_{ow}: 2.27 (EPI Suite)</p> <p>Molecular Weight: 133.15</p> <p>Vapor Pressure: 0.238 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1038 mg/L (EPI Suite)</p>	<p>2-Methyl-1,3-benzoxazole</p> <p>2-Methyl-4,5-benzoxazole</p> <p>2-Methylbenzoxazol</p> <p>2-Methylbenzoxazole</p> <p>Benzoxazole, 2-methyl-</p>	 <p>The structure shows a benzene ring fused to a five-membered benzoxazole ring. A methyl group (H₃C) is attached to the 2-position of the benzoxazole ring.</p>

Table 1: Material Identification

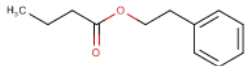
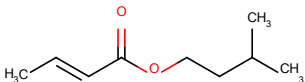
Material	Synonyms	Structure
<p>α-Methylbenzyl butyrate</p> <p>C₁₂H₁₆O₂</p> <p>CAS # 3460-44-4</p> <p>Log K_{ow}: 3.55 (EPI Suite)</p> <p>Molecular Weight: 192.25</p> <p>Vapor Pressure: 0.00859 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 44.15 mg/L (EPI Suite)</p>	<p>α-Methylbenzyl butyrate</p> <p>1-Phenyl-1-ethyl butanoate</p> <p>1-Phenylethyl butyrate</p> <p>Butanoic acid, 1-phenylethyl ester</p> <p>Methyl phenylcarbonyl butyrate</p> <p>Styralyl butyrate</p>	 <p>The structure shows a butyrate chain (CH₃-CH₂-CH₂-C(=O)-O-) attached to a 1-phenylethyl group (-CH(CH₃)-C₆H₅).</p>
<p>3-Methylbutyl 2-butenate</p> <p>C₉H₁₆O₂</p> <p>CAS # 25415-77-4</p> <p>Log K_{ow}: 3.03 (EPI Suite)</p> <p>Molecular Weight: 156.22</p> <p>Vapor Pressure: 0.528 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 183.6 mg/L (EPI Suite)</p>	<p>2-Butenoic acid, 3-methylbutyl ester</p> <p>3-Methylbutyl 2-butenate</p> <p>3-Methylbutyl but-2-enoate</p> <p>Isoamyl 2-butenate</p> <p>Isoamyl crotonate</p> <p>Isopentyl 2-butenate</p>	 <p>The structure shows a 2-butenate chain (H₃C-CH=CH-C(=O)-O-) attached to a 3-methylbutyl group (-CH₂-CH₂-CH₂-CH(CH₃)-CH₃).</p>

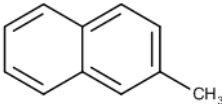
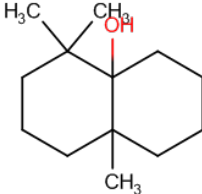
Table 1: Material Identification		
Material	Synonyms	Structure
<p>2-Methylnaphthalene</p> <p>C₁₁H₁₀</p> <p>CAS # 91-57-6</p> <p>Log K_{ow}: 3.72 (EPI Suite)</p> <p>Molecular Weight: 142.2</p> <p>Vapor Pressure: 0.0201 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 41.42 mg/L (EPI Suite)</p>	<p>2-Methylnaphthalene</p> <p>2-メチルナフタレン</p> <p>Naphthalene, 2-methyl-</p>	
<p>4a(2H)-Naphthalenol, octahydro-4,4,8a-trimethyl-, cis-</p> <p>C₁₃H₂₄O</p> <p>CAS # 57963-77-6</p> <p>Log K_{ow}: 4.02 (EPI Suite)</p> <p>Molecular Weight: 196.33</p> <p>Vapor Pressure: 0.000473 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 54.68 mg/L (EPI Suite)</p>	<p><i>cis</i>-Octahydro-4,4,8a-trimethyl-4a(2H)-naphthalenol</p> <p>4a(2H)-Naphthalenol, octahydro-4,4,8a-trimethyl-, <i>cis</i>-</p> <p>Methyl geosmin</p>	

Table 1: Material Identification

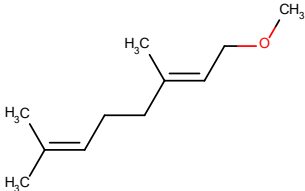
Material	Synonyms	Structure
<p data-bbox="485 321 720 345">Neryl methyl ether</p> <p data-bbox="554 380 651 404">C₁₁H₂₀O</p> <p data-bbox="243 500 453 524">CAS # 2565-83-5</p> <p data-bbox="243 623 541 647">Log K_{ow}: 4.17 (EPI Suite)</p> <p data-bbox="243 683 548 708">Molecular Weight: 168.28</p> <p data-bbox="243 743 842 768">Vapor Pressure: 0.356 mm Hg @ 25°C (EPI Suite)</p> <p data-bbox="243 803 716 828">Water Solubility: 17.23 mg/L (EPI Suite)</p> <p data-bbox="243 927 789 951">*Additional Material for Main CAS # 2565-82-4</p>	<p data-bbox="1001 500 1493 524">(Z)-1-Methoxy-3,7-dimethylocta-2,6-diene</p> <p data-bbox="1022 560 1472 584">1-Methoxy-3,7-dimethylocta-2,6-diene</p> <p data-bbox="1005 620 1484 644">2,6-Octadiene, 1-methoxy-3,7-dimethyl-,</p> <p data-bbox="1224 680 1266 704">(Z)-</p> <p data-bbox="1136 740 1354 764">Neryl methyl ether</p>	 <p>The chemical structure shows a zigzag carbon chain with two double bonds in a (Z) configuration. The first double bond is at the 2-position, with two methyl groups (H₃C) attached. The second double bond is at the 6-position, with a methyl group (H₃C) and a methoxy group (-OCH₃) attached. The methoxy group is highlighted in red.</p>

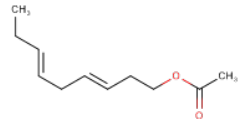
Table 1: Material Identification		
Material	Synonyms	Structure
<p>3,6-Nonadien-1-ol,1-acetate</p> <p>C₁₁H₁₈O₂</p> <p>CAS # 76649-26-8</p> <p>Log K_{ow}: 3.87 (EPI Suite)</p> <p>Molecular Weight: 182.26</p> <p>Vapor Pressure: 0.0441 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 26.5 mg/L (EPI Suite)</p>	<p>3,6-Nonadien-1-ol, 1-acetate</p> <p>3,6-Nonadienyl acetate</p>	

Table 1: Material Identification		
Material	Synonyms	Structure
<p>(E,Z)-3,6-Nonadien-1-ol acetate</p> <p>C₁₁H₁₈O₂</p> <p>CAS # 211323-05-6</p> <p>Log K_{ow}:</p> <p>Molecular Weight: 182.26</p> <p>Vapor Pressure:</p> <p>Water Solubility:</p> <p>*Additional Material for Main CAS # 76649-26-8</p>	<p>(E,Z)-3,6-Nonadien-1-ol acetate</p> <p><i>trans</i>-3-<i>cis</i>-6-Nonadien-1-yl acetate</p>	

Table 1: Material Identification		
Material	Synonyms	Structure
<p>2,6-Nonadienal diethyl acetal</p> <p>C₁₃H₂₄O₂</p> <p>CAS # 67674-36-6</p> <p>Log K_{ow}: 4.21 (EPI Suite)</p> <p>Molecular Weight: 212.33</p> <p>Vapor Pressure: 0.0151 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 9.542 mg/L (EPI Suite)</p>	<p>(2E,6Z)-1,1-Diethoxynona-2,6-diene</p> <p>1,1-Diethoxynona-2,6-diene</p> <p>2,6-Nonadienal diethyl acetal</p> <p>2,6-Nonadiene, 1,1-diethoxy-, (E,Z)-</p>	

Table 1: Material Identification

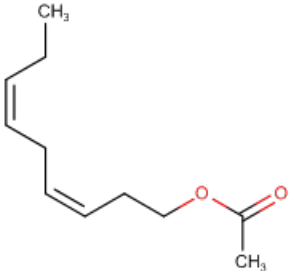
Material	Synonyms	Structure
<p><i>cis,cis-3,6-Nonadienyl acetate</i></p> <p>C₁₁H₁₈O₂</p> <p>CAS # 83334-93-4</p> <p>Log K_{ow}: 182.26 (EPI Suite)</p> <p>Molecular Weight: 182.26</p> <p>Vapor Pressure: 0.0441 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 26.5 mg/L (EPI Suite)</p> <p>*Additional Material for Main CAS # 76649-26-8</p>	<p>(Z,Z)-3,6-Nonadienyl acetate</p> <p><i>cis,cis-3,6-Nonadienyl acetate</i></p> <p>3,6-Nonadien-1-ol, acetate, (3Z,6Z)-</p> <p>Acetic acid, (Z,Z)-3,6-nonadienyl ester</p>	

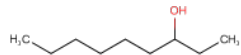
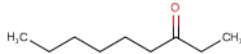
Table 1: Material Identification		
Material	Synonyms	Structure
<p>3-Nonanol</p> <p>$C_9H_{20}O$</p> <p>CAS # 624-51-1</p> <p>Log K_{ow}: 3.22 (EPI Suite)</p> <p>Molecular Weight: 144.25</p> <p>Vapor Pressure: 0.0404 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 459.7 mg/L (EPI Suite)</p>	<p>3-Nonanol</p> <p>Nonan-3-ol</p>	
<p>3-Nonanone</p> <p>$C_9H_{20}O$</p> <p>CAS # 925-78-0</p> <p>Log K_{ow}: 2.71 (EPI Suite)</p> <p>Molecular Weight: 142.24</p> <p>Vapor Pressure: 0.58 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 396.1 mg/L (EPI Suite)</p>	<p>3-Nonanone</p> <p>Ethyl hexyl ketone</p> <p>Nonan-3-one</p>	

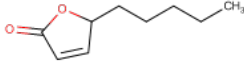
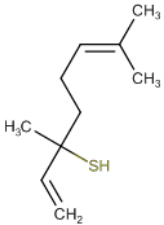
Table 1: Material Identification		
Material	Synonyms	Structure
<p>2-Nonenoic acid γ-lactone</p> <p>$C_9H_{14}O_2$</p> <p>CAS # 21963-26-8</p> <p>Log K_{ow}: 1.86 (EPI Suite)</p> <p>Molecular Weight: 154.20</p> <p>Vapor Pressure: 0.0105 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 1871 mg/L (EPI Suite)</p>	<p>2-Nonenoic acid γ-lactone</p> <p>2-Nonenoic acid, 4-hydroxy-, γ-lactone</p> <p>2(5H)-Furanone, 5-pentyl-</p> <p>5-Pentyl-5H-furan-2-one</p> <p>5-Pentylfuran-2(5H)-one</p>	
<p>1,6-Octadiene-3-thiol, 3,7-dimethyl-</p> <p>$C_{10}H_{18}S$</p> <p>CAS # 39707-47-6</p> <p>Log K_{ow}: 4.79 (EPI Suite)</p> <p>Molecular Weight: 170.31</p> <p>Vapor Pressure: 0.178 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 4.976 mg/L (EPI Suite)</p>	<p>1,6-Octadiene-3-thiol, 3,7-dimethyl-</p> <p>3,7-Dimethyl-1,6-octadiene-3-thiol</p>	

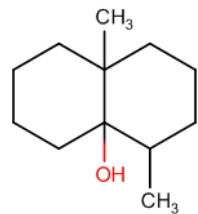
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Octahydro-4,8a-dimethyl-4a(2H)-naphthol</p> <p>C₁₂H₂₂O</p> <p>CAS # 23333-91-7</p> <p>Log K_{ow}: 3.57 (EPI Suite)</p> <p>Molecular Weight: 182.30</p> <p>Vapor Pressure: 0.000289 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 156.7 mg/L (EPI Suite)</p>	<p>1,10-Dimethyl-9-decalol</p> <p>4,8a-Dimethyloctahydronaphthalen-4a(2H)-ol</p> <p>4a(2H)-Naphthalenol, octahydro-4,8a-dimethyl-</p> <p>Geosmin</p> <p>Octahydro-4,8a-dimethyl-4a(2H)-naphthol</p>	

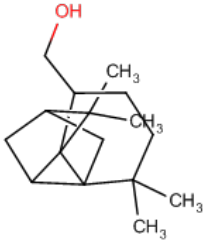
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Octahydro-7,7,8,8-tetramethyl-2,3b-methano-3bH-cyclopenta[1,3]cyclopropa[1,2]benzene-4-methanol</p> <p>C₁₆H₂₆O</p> <p>CAS # 59056-64-3</p> <p>Log K_{ow}: 4.59 (EPI Suite)</p> <p>Molecular Weight: 234.38</p> <p>Vapor Pressure: 0.0000138 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 11.14 mg/L (EPI Suite)</p>	<p>(7,7,8,8-Tetramethyloctahydro-2,3b-methanocyclopenta[1,3]cyclopropa[1,2]benzen-4-yl)methanol</p> <p>2,3b-Methano-3bH-cyclopenta[1,3]cyclopropa[1,2]benzene-4-methanol, octahydro-7,7,8,8-tetramethyl-Octahydro-7,7,8,8-tetramethyl-2,3b-methano-3bH-cyclopenta[1,3]cyclopropa[1,2]benzene-4-methanol</p>	

Table 1: Material Identification

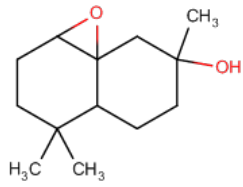
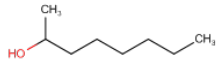
Material	Synonyms	Structure
<p>Octahydro-4,4,7-trimethyl-3H-naphth[1,8a-b]oxiren-7-ol</p> <p>$C_{13}H_{22}O_2$</p> <p>CAS # 68845-01-2</p> <p>Log K_{ow}: 2.5 (EPI Suite)</p> <p>Molecular Weight: 210.31</p> <p>Vapor Pressure: 0.000125 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 913.1 mg/L (EPI Suite)</p>	<p>3H-Naphth[1,8a-b]oxiren-7-ol, octahydro-4,4,7-trimethyl-8,8a-Epoxy-decahydro-2,5,5-trimethyl-2-naphthol</p> <p>Ambrinoloxyde</p> <p>Octahydro-4,4,7-trimethyl-3H-naphth[1,8a-b]oxiren-7-ol</p>	 <p>The structure shows a bicyclic system consisting of two fused six-membered rings. The bridgehead oxygen atom is highlighted in red. The right-hand ring has a methyl group (CH₃) and a hydroxyl group (OH) attached to the same carbon atom. The left-hand ring has two methyl groups (H₃C and CH₃) attached to the same carbon atom.</p>
<p>2-Octanol</p> <p>$C_8H_{18}O$</p> <p>CAS # 123-96-6</p> <p>Log K_{ow}: 2.73 (EPI Suite)</p> <p>Molecular Weight: 130.23</p> <p>Vapor Pressure: 0.156 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 990.9 mg/L (EPI Suite)</p>	<p><i>sec</i>-Capryl alcohol</p> <p><i>sec</i>-Caprylic alcohol</p> <p><i>sec</i>-Octyl alcohol</p> <p>2-Octanol</p> <p>Hexyl methyl carbinol</p> <p>Methyl hexyl carbinol</p> <p>Octan-2-ol</p>	 <p>The structure shows a straight-chain eight-carbon alkane with a hydroxyl group (HO) attached to the second carbon atom. A methyl group (CH₃) is attached to the third carbon atom.</p>

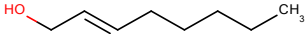
Table 1: Material Identification		
Material	Synonyms	Structure
<p>2-Octen-1-ol</p> <p>C₈H₁₆O</p> <p>CAS # 22104-78-5</p> <p>Log K_{ow}: 2.59 (EPI Suite)</p> <p>Molecular Weight: 128.21</p> <p>Vapor Pressure: 0.049 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 1855 mg/L (EPI Suite)</p> <p>*Additional Material for Main CAS # 18409-17-1</p>	<p>2-Octen-1-ol</p>	

Table 1: Material Identification

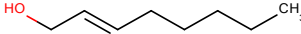
Material	Synonyms	Structure
<p data-bbox="499 321 701 347">(E)-2-Octen-1-ol</p> <p data-bbox="558 380 642 406">C₈H₁₆O</p> <p data-bbox="243 500 464 526">CAS # 18409-17-1</p> <p data-bbox="243 623 541 649">Log K_{ow}: 2.59 (EPI Suite)</p> <p data-bbox="243 682 548 708">Molecular Weight: 128.21</p> <p data-bbox="243 740 842 766">Vapor Pressure: 0.049 mm Hg @ 25°C (EPI Suite)</p> <p data-bbox="369 799 831 824">Water Solubility: 1855 mg/L (EPI Suite)</p>	<p data-bbox="1146 438 1346 464">(E)-2-Octen-1-ol</p> <p data-bbox="1136 496 1356 522"><i>trans</i>-2-Octen-1-ol</p> <p data-bbox="1163 555 1329 581">2-(E)-Octenol</p> <p data-bbox="1142 613 1350 639">2-Octen-1-ol, (E)-</p> <p data-bbox="1163 672 1329 698">Oct-2-en-1-ol</p>	 <p>The image shows the skeletal structure of (E)-2-Octen-1-ol. It consists of an eight-carbon chain. The first carbon is bonded to a hydroxyl group (HO) and a hydrogen atom. The second carbon is part of a double bond with the third carbon, and the two groups on the double bond are on opposite sides (E configuration). The chain continues to the eighth carbon, which is bonded to three hydrogen atoms (CH₃).</p>

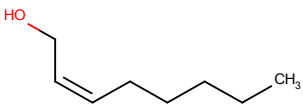
Table 1: Material Identification		
Material	Synonyms	Structure
<p><i>cis</i>-2-Octenol</p> <p>C₈H₁₆O</p> <p>CAS # 26001-58-1</p> <p>Log K_{ow}: 2.59 (EPI Suite)</p> <p>Molecular Weight: 128.21</p> <p>Vapor Pressure: 0.049 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 1855 mg/L (EPI Suite)</p> <p>*Additional Material for Main CAS # 18409-17-1</p>	<p>(Z)-2-Octen-1-ol</p> <p><i>cis</i>-2-Octen-1-ol</p> <p><i>cis</i>-2-Octenol</p>	 <p>The structure shows a zigzag carbon chain with a double bond between the second and third carbons. The hydroxyl group (HO) is attached to the first carbon, and a methyl group (CH₃) is attached to the eighth carbon. The double bond is in the Z configuration.</p>

Table 1: Material Identification

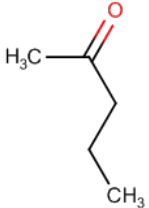
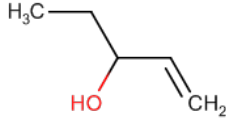
Material	Synonyms	Structure
<p>2-Pentanone</p> <p>C₅H₁₀O</p> <p>CAS # 107-87-9</p> <p>Log K_{ow}: 0.75 (EPI Suite)</p> <p>Molecular Weight: 86.13</p> <p>Vapor Pressure: 30.5 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 21230 mg/L (EPI Suite)</p>	<p>2-Pentanone</p> <p>Ethyl acetone</p> <p>Methyl propyl ketone</p> <p>Pentan-2-one</p> <p>Propyl methyl ketone</p>	 <p>The structure shows a five-carbon chain with a carbonyl group (C=O) at the second carbon. The first carbon is a methyl group (H₃C) and the fifth carbon is also a methyl group (CH₃).</p>
<p>1-Penten-3-ol</p> <p>C₅H₁₀O</p> <p>CAS # 616-25-1</p> <p>Log K_{ow}: 1.12 (EPI Suite)</p> <p>Molecular Weight: 86.13</p> <p>Vapor Pressure: 6.47 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 45260 mg/L (EPI Suite)</p>	<p>1-Penten-3-ol</p> <p>Ethyl vinyl carbinol</p> <p>Pent-1-en-3-ol</p> <p>Vinyl ethyl carbinol</p>	 <p>The structure shows a five-carbon chain with a hydroxyl group (HO) at the third carbon and a vinyl group (CH=CH₂) at the first carbon. The fifth carbon is a methyl group (H₃C).</p>

Table 1: Material Identification

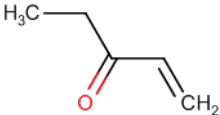
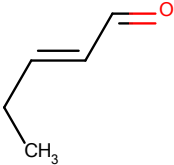
Material	Synonyms	Structure
<p>1-Penten-3-one</p> <p>C₅H₈O</p> <p>CAS # 1629-58-9</p> <p>Log K_{ow}: 0.9 (EPI Suite)</p> <p>Molecular Weight: 84.11</p> <p>Vapor Pressure: 29.5 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 21900 mg/L (EPI Suite)</p>	<p>1-Penten-3-one</p> <p>Ethyl vinylketone</p> <p>Pent-1-en-3-one</p>	 <p>The structure shows a five-carbon chain. The third carbon from the left is a carbonyl group (C=O). The first carbon is a methyl group (H₃C). The fifth carbon is a terminal vinyl group (CH₂).</p>
<p>2-Pentenal</p> <p>C₅H₈O</p> <p>CAS # 764-39-6</p> <p>Log K_{ow}: 1.09 (EPI Suite)</p> <p>Molecular Weight: 84.11</p> <p>Vapor Pressure: 13.9 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 14980 mg/L (EPI Suite)</p>	<p>2-Pentenal</p> <p>3-Ethyl-2-propenal</p> <p>3-Ethylacrolein</p> <p>Pent-2-enal</p>	 <p>The structure shows a five-carbon chain. The second carbon from the left is a double bond. The first carbon is a methyl group (CH₃). The fifth carbon is an aldehyde group (C=O).</p>

Table 1: Material Identification

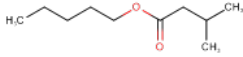
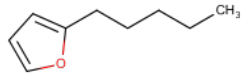
Material	Synonyms	Structure
<p>Pentyl isovalerate</p> <p>C₁₀H₂₀O₂</p> <p>CAS # 25415-62-7</p> <p>Log K_{ow}: 3.74 (EPI Suite)</p> <p>Molecular Weight: 172.26</p> <p>Vapor Pressure: 0.39 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 38.59 mg/L (EPI Suite)</p>	<p>Amyl 3-methylbutanoate</p> <p>Amyl isovalerate</p> <p>Butanoic acid, 3-methyl-, pentyl ester</p> <p>Pentyl 3-methylbutanoate</p> <p>Pentyl isovalerate</p> <p>ペンタン酸アルキル(C=1~5)</p>	 <p>The structure shows a pentyl chain (H₃C-CH₂-CH₂-CH₂-CH₂-O-) attached to the oxygen of an ester group. The ester group is attached to a 3-methylbutanoate chain (-C(=O)-CH₂-CH(CH₃)-CH₃).</p>
<p>2-Pentylfuran</p> <p>C₉H₁₄O</p> <p>CAS # 3777-69-3</p> <p>Log K_{ow}: 3.87 (EPI Suite)</p> <p>Molecular Weight: 138.21</p> <p>Vapor Pressure: 0.837 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 41.84 mg/L (EPI Suite)</p>	<p>2-Amylfuran</p> <p>2-Pentylfuran</p> <p>Furan, 2-pentyl-</p>	 <p>The structure shows a furan ring with an oxygen atom at the bottom position. A pentyl chain (-CH₂-CH₂-CH₂-CH₂-CH₃) is attached to the 2-position of the furan ring.</p>

Table 1: Material Identification		
Material	Synonyms	Structure
<p>Pentylpropionate</p> <p>$C_8H_{16}O_2$</p> <p>CAS # 624-54-4</p> <p>Log K_{ow}: 2.83 (EPI Suite)</p> <p>Molecular Weight: 144.21</p> <p>Vapor Pressure: 1.18 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 308.7 mg/L (EPI Suite)</p>	<p>Amyl propionate</p> <p>Pentyl propionate</p> <p>Propanoic acid, pentyl ester</p>	
<p>Phenol, 4-butyl-</p> <p>$C_{10}H_{14}O$</p> <p>CAS # 1638-22-8</p> <p>Log K_{ow}: 3.53 (EPI Suite)</p> <p>Molecular Weight: 150.22</p> <p>Vapor Pressure: 0.00782 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 219.8 mg/L (EPI Suite)</p>	<p>Phenol, 4-butyl-</p>	

Table 1: Material Identification

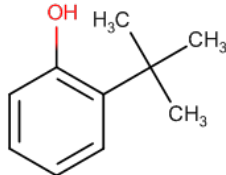
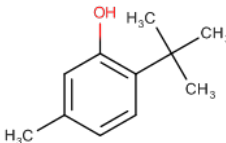
Material	Synonyms	Structure
<p>Phenol, 2-(1,1-dimethylethyl)-</p> <p>C₁₀H₁₄O</p> <p>CAS # 88-18-6</p> <p>Log K_{ow}: 3.42 (EPI Suite)</p> <p>Molecular Weight: 150.22</p> <p>Vapor Pressure: 0.0337 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 428.9 mg/L (EPI Suite)</p>	<p>Phenol, 2-(1,1-dimethylethyl)-</p>	 <p>The structure shows a benzene ring with a hydroxyl group (OH) at the top position. At the ortho position (position 2), there is a tert-butyl group, which is a central carbon atom bonded to three methyl groups (CH₃).</p>
<p>Phenol, 2-(1,1-dimethylethyl)-5-methyl-</p> <p>C₁₁H₁₆O</p> <p>CAS # 88-60-8</p> <p>Log K_{ow}: 3.97 (EPI Suite)</p> <p>Molecular Weight: 164.24</p> <p>Vapor Pressure: 0.00443 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 101.3 mg/L (EPI Suite)</p>	<p>6-<i>tert</i>-Butyl-<i>m</i>-cresol</p> <p>Phenol, 2-(1,1-dimethylethyl)-5-methyl-</p>	 <p>The structure shows a benzene ring with a hydroxyl group (OH) at the top position. At the ortho position (position 2), there is a tert-butyl group. At the meta position (position 5), there is a methyl group (H₃C).</p>

Table 1: Material Identification

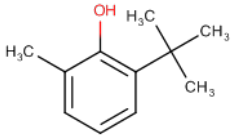
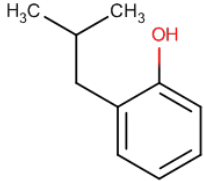
Material	Synonyms	Structure
<p>Phenol, 2-(1,1-dimethylethyl)-6-methyl-</p> <p>C₁₁H₁₆O</p> <p>CAS # 2219-82-1</p> <p>Log K_{ow}: 3.97 (EPI Suite)</p> <p>Molecular Weight: 164.24</p> <p>Vapor Pressure: 0.0169 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 101.3 mg/L (EPI Suite)</p>	<p>Phenol, 2-(1,1-dimethylethyl)-6-methyl-</p>	 <p>The structure shows a benzene ring with a hydroxyl group (OH) at the 1-position, a methyl group (H₃C) at the 6-position, and a 1,1-dimethylethyl group (a central carbon bonded to two methyl groups and one ethyl group) at the 2-position.</p>
<p>Phenol, (2-methylpropyl)-</p> <p>C₁₀H₁₄O</p> <p>CAS # 31195-95-6</p> <p>Log K_{ow}: 3.46 (EPI Suite)</p> <p>Molecular Weight: 150.22</p> <p>Vapor Pressure: 0.00973 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 319.4 mg/L (EPI Suite)</p>	<p>Phenol, (2-methylpropyl)-</p>	 <p>The structure shows a benzene ring with a hydroxyl group (OH) at the 1-position and a 2-methylpropyl group (a propyl chain with a methyl group on the second carbon) at the 2-position.</p>

Table 1: Material Identification

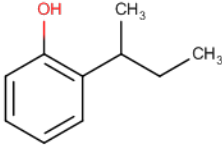
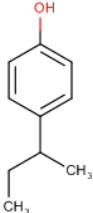
Material	Synonyms	Structure
<p>Phenol, 2-(1-methylpropyl)-</p> <p>C₁₁H₁₄O</p> <p>CAS # 89-72-5</p> <p>Log K_{ow}: 3.46 (EPI Suite)</p> <p>Molecular Weight: 150.22</p> <p>Vapor Pressure: 0.0252 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 464 mg/L (EPI Suite)</p>	<p><i>ortho-sec</i>-Butylphenol</p> <p>2-(1-Methylpropyl)phenol</p> <p>2-<i>sec</i>-Butylphenol</p> <p>Phenol, 2-(1-methylpropyl)-</p>	 <p>The structure shows a benzene ring with a hydroxyl group (OH) at the top position. At the ortho position (bottom-left), there is a 1-methylpropyl group. The methyl group is labeled CH₃, and the propyl chain is shown as a zigzag line ending in another CH₃ group.</p>
<p>Phenol, 4-(1-methylpropyl)-</p> <p>C₁₁H₁₄O</p> <p>CAS # 99-71-8</p> <p>Log K_{ow}: 3.46 (EPI Suite)</p> <p>Molecular Weight: 150.22</p> <p>Vapor Pressure: 0.00462 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 674.2 mg/L (EPI Suite)</p>	<p>Phenol, 4-(1-methylpropyl)-</p>	 <p>The structure shows a benzene ring with a hydroxyl group (OH) at the top position. At the para position (bottom), there is a 1-methylpropyl group. The methyl group is labeled CH₃, and the propyl chain is shown as a zigzag line ending in another CH₃ group.</p>

Table 1: Material Identification

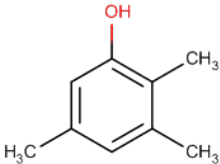
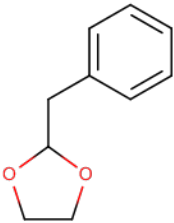
Material	Synonyms	Structure
<p>Phenol, 2,3,5-trimethyl-</p> <p>C₉H₁₂O</p> <p>CAS # 697-82-5</p> <p>Log K_{ow}: 3.15 (EPI Suite)</p> <p>Molecular Weight: 136.19</p> <p>Vapor Pressure: 0.0039 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 667.6 mg/L (EPI Suite)</p>	<p>Phenol, 2,3,5-trimethyl-</p>	 <p>The structure shows a benzene ring with a hydroxyl group (OH) at the top position (1) and methyl groups (CH₃) at the 2, 3, and 5 positions. The methyl group at the 3-position is labeled H₃C.</p>
<p>Phenylacetaldehyde ethylene glycol acetal</p> <p>C₁₀H₁₂O₂</p> <p>CAS # 101-49-5</p> <p>Log K_{ow}: 1.82 (EPI Suite)</p> <p>Molecular Weight: 164.20</p> <p>Vapor Pressure: 0.0217 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1834 mg/L (EPI Suite)</p>	<p>1,3-Dioxolane, 2-(phenylmethyl)-</p> <p>2-Benzyl-1,3-dioxolane</p> <p>2-Benzylidioxolan</p> <p>Phenylacetaldehyde ethylene glycol acetal</p>	 <p>The structure shows a five-membered 1,3-dioxolane ring with a benzyl group (a methylene group attached to a benzene ring) at the 2-position.</p>

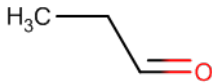
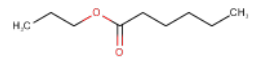
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Propionaldehyde</p> <p>C₃H₆O</p> <p>CAS # 123-38-6</p> <p>Log K_{ow}: 0.33 (EPI Suite)</p> <p>Molecular Weight: 58.08</p> <p>Vapor Pressure: 256 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 42990 mg/L (EPI Suite)</p>	<p>Methylacetaldehyde</p> <p>Propanal</p> <p>Propionaldehyde</p> <p>Propyl aldehyde</p> <p>プロピオンアルデヒド</p>	
<p>Propyl hexanoate</p> <p>C₉H₁₈O₂</p> <p>CAS # 626-77-7</p> <p>Log K_{ow}: 3.32 (EPI Suite)</p> <p>Molecular Weight: 158.24</p> <p>Vapor Pressure: 0.473 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 101.9 mg/L (EPI Suite)</p>	<p>Hexanoic acid, propyl ester</p> <p>Propyl caproate</p> <p>Propyl hexanoate</p>	

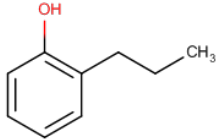
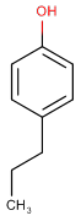
Table 1: Material Identification		
Material	Synonyms	Structure
<p><i>o</i>-Propylphenol</p> <p>C₉H₁₂O</p> <p>CAS # 644-35-9</p> <p>Log K_{ow}: 3.04 (EPI Suite)</p> <p>Molecular Weight: 136.19</p> <p>Vapor Pressure: 0.04 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1039 mg/L (EPI Suite)</p>	<p><i>o</i>-Propylphenol</p> <p>1-(2-Hydroxyphenyl)propane</p> <p>2-Propylphenol</p> <p>Phenol, 2-propyl-</p>	
<p><i>p</i>-Propylphenol</p> <p>C₉H₁₂O</p> <p>CAS # 645-56-7</p> <p>Log K_{ow}: 3.04 (EPI Suite)</p> <p>Molecular Weight: 136.19</p> <p>Vapor Pressure: 0.0193 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 610.7 mg/L (EPI Suite)</p>	<p><i>p</i>-Propylphenol</p> <p>4-Propylphenol</p> <p>Dihydrochavicol</p> <p>Dihydrojonquitol</p> <p>Phenol, 4-propyl-</p>	

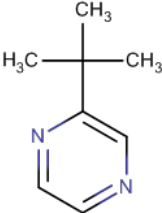
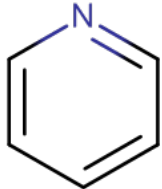
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Pyrazine, (1,1-dimethylethyl)-</p> <p>C₈H₁₂N₂</p> <p>CAS # 32741-11-0</p> <p>Log K_{ow}: 1.85 (EPI Suite)</p> <p>Molecular Weight: 136.19</p> <p>Vapor Pressure: 0.417 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 2286 mg/L (EPI Suite)</p>	<p><i>tert</i>-Butylpyrazine</p> <p>2-<i>tert</i>-Butylpyrazine</p> <p>Pyrazine, (1,1-dimethylethyl)-</p>	
<p>Pyridine</p> <p>C₅H₅N</p> <p>CAS # 110-86-1</p> <p>Log K_{ow}: 0.8 (EPI Suite)</p> <p>Molecular Weight: 79.10</p> <p>Vapor Pressure: 14.5 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 729800 mg/L (EPI Suite)</p>	<p>Azine</p> <p>Pyridine</p>	

Table 1: Material Identification

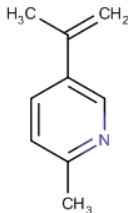
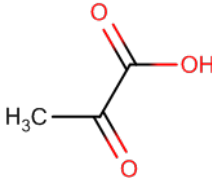
Material	Synonyms	Structure
<p>Pyridine, 2-methyl-5-(1-methylethenyl)-</p> <p>C₉H₁₁N</p> <p>CAS # 56057-93-3</p> <p>Log K_{ow}: 2.8 (EPI Suite)</p> <p>Molecular Weight: 133.19</p> <p>Vapor Pressure: 0.345 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 362 mg/L (EPI Suite)</p>	<p>2-Methyl-5-isopropenylpyridine</p> <p>2-Picoline, 5-isopropenyl</p> <p>5-Isopropenyl-2-methylpyridine</p> <p>Pyridine, 2-methyl-5-(1-methylethenyl)-</p>	 <p>The structure shows a pyridine ring with a methyl group (CH₃) at the 2-position and a 1-methylethenyl group (CH₂=C(CH₃)-) at the 5-position.</p>
<p>Pyruvic acid</p> <p>C₃H₄O₃</p> <p>CAS # 127-17-3</p> <p>Log K_{ow}: -1.24 (EPI Suite)</p> <p>Molecular Weight: 88.06</p> <p>Vapor Pressure: 0.478 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1e+006 mg/L (EPI Suite)</p>	<p>α-Ketopropionic acid</p> <p>2-Ketopropionic acid</p> <p>2-Oxopropanoic acid</p> <p>Acetylformic acid</p> <p>Propanoic acid, 2-oxo-</p> <p>Pyroracemic acid</p> <p>Pyruvic acid</p>	 <p>The structure shows a three-carbon chain with a methyl group (H₃C) at the end, a carbonyl group (C=O) at the second carbon, and a carboxylic acid group (C(=O)OH) at the first carbon.</p>

Table 1: Material Identification

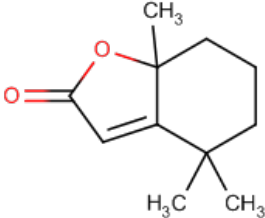
Material	Synonyms	Structure
<p data-bbox="531 472 672 496">Tealactone</p> <p data-bbox="548 532 655 557">C₁₁H₁₆O₂</p> <p data-bbox="243 654 466 678">CAS # 15356-74-8</p> <p data-bbox="243 776 525 800">Log K_{ow}: 2.3 (EPI Suite)</p> <p data-bbox="243 837 548 862">Molecular Weight: 180.24</p> <p data-bbox="243 899 945 924">Vapor Pressure: 0.000958 mm Hg @ 20°C (EPI Suite v4.0)</p> <p data-bbox="243 961 714 985">Water Solubility: 600.6 mg/L (EPI Suite)</p>	<p data-bbox="1100 321 1392 345">(±) Dihydroactinidiolide</p> <p data-bbox="1104 383 1388 407">(±)-(2,6,6-Trimethyl-2-</p> <p data-bbox="1024 444 1465 469">hydroxycyclohexylidene)acetic acid γ-</p> <p data-bbox="1203 506 1289 531">lactone</p> <p data-bbox="1136 568 1356 592">(2,6,6-Trimethyl-2-</p> <p data-bbox="1031 630 1461 654">hydroxycyclohexylidene)acetic acid</p> <p data-bbox="1203 691 1289 716">lactone</p> <p data-bbox="995 753 1497 777">2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-</p> <p data-bbox="1150 815 1344 839">4,4,7a-trimethyl-</p> <p data-bbox="1016 876 1478 901">4,4,7a-Trimethyl-5,6,7,7a-tetrahydro-1-</p> <p data-bbox="1115 938 1379 963">benzofuran-2(4H)-one</p> <p data-bbox="1031 1000 1463 1024">4,5,7,7a-Tetrahydro-4,4,7a-trimethyl-</p> <p data-bbox="1123 1062 1371 1086">2(6H)benzofuranone</p> <p data-bbox="1178 1123 1316 1148">Tealactone</p>	 <p>The chemical structure of Tealactone is a bicyclic lactone. It consists of a benzofuranone core with a cyclohexane ring fused to the furanone ring. The furanone ring has a carbonyl group at position 2 and a double bond between positions 3 and 4. The cyclohexane ring has a methyl group at position 6 and two methyl groups at position 7a. The oxygen atom in the furanone ring is highlighted in red in the original image.</p>

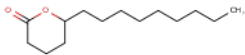
Table 1: Material Identification		
Material	Synonyms	Structure
<p>δ-Tetradecalactone</p> <p>C₁₄H₂₆O₂</p> <p>CAS # 2721-22-4</p> <p>Log K_{ow}: 4.53 (EPI Suite)</p> <p>Molecular Weight: 226.36</p> <p>Vapor Pressure: 0.0000927 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 4.294 mg/L (EPI Suite)</p>	<p>δ-Tetradecalactone</p> <p>2H-Pyran-2-one, tetrahydro-6-nonyl-</p> <p>5-Hydroxytetradecanoic acid lactone</p> <p>6-Nonyltetrahydro-2H-pyran-2-one</p> <p>Tetradeca-1,5-lactone</p>	

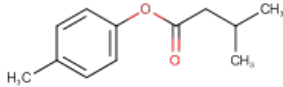
Table 1: Material Identification		
Material	Synonyms	Structure
<p><i>p</i>-Tolyl 3-methylbutyrate</p> <p>C₁₂H₁₆O₂</p> <p>CAS # 55066-56-3</p> <p>Log K_{ow}: 3.54 (EPI Suite)</p> <p>Molecular Weight: 192.25</p> <p>Vapor Pressure: 0.00904 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 45.68 mg/L (EPI Suite)</p>	<p>-Cresyl 3-methylbutanoate</p> <p><i>p</i>-Cresyl isovalerate</p> <p><i>p</i>-Methylphenyl 3-methylbutyrate</p> <p><i>p</i>-Tolyl 3-methylbutyrate</p> <p><i>p</i>-Tolyl isovalerate</p> <p>4-Methylphenyl 3-methylbutanoate</p> <p>Butanoic acid, 3-methyl-, 4-methylphenyl ester</p> <p>アルキル (C = 1 ~ 7) カルボン酸クレジ ル</p>	


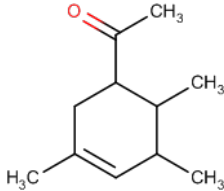
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Tridecane</p> <p>$C_{13}H_{28}$</p> <p>CAS # 629-50-5</p> <p>Log K_{ow}: 6.73 (EPI Suite)</p> <p>Molecular Weight: 184.36</p> <p>Vapor Pressure: 0.0607 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 0.02746 mg/L (EPI Suite)</p>	<p>Tridecane</p> <p>アルカン(C 10~29)</p>	
<p>1-(3,5,6-Trimethyl-3-cyclohexen-1-yl)ethan-1-one</p> <p>$C_{11}H_{16}O$</p> <p>CAS # 68480-14-8</p> <p>Log K_{ow}: 3.2 (EPI Suite)</p> <p>Molecular Weight: 166.26</p> <p>Vapor Pressure: 0.118 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 118 mg/L (EPI Suite)</p>	<p>1-(3,5,6-Trimethyl-3-cyclohexen-1-yl)ethan-1-one</p> <p>1-(3,5,6-Trimethylcyclohex-3-en-1-yl)ethanone</p> <p>Ethanone, 1-(3,5,6-trimethyl-3-cyclohexen-1-yl)-</p> <p>Methyl Cyclo Citrone</p>	

Table 1: Material Identification

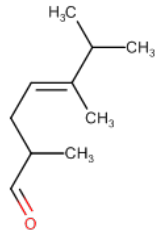
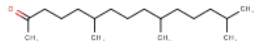
Material	Synonyms	Structure
<p>2,5,6-Trimethyl-4-heptenal</p> <p>C₁₀H₁₈O</p> <p>CAS # 82784-84-7</p> <p>Log K_{ow}: 3.46 (EPI Suite)</p> <p>Molecular Weight: 154.25</p> <p>Vapor Pressure: 0.51 mm Hg @ 25°C (EPI Suite)</p> <p>Water Solubility: 81.1 mg/L (EPI Suite)</p>	<p>2,5,6-Trimethyl-4-hepten-1-al</p> <p>2,5,6-Trimethyl-4-heptenal</p> <p>2,5,6-Trimethylhept-4-enal</p> <p>Greenal</p>	 <p>The structure shows a seven-carbon chain with an aldehyde group at C1, a double bond between C4 and C5, and methyl groups at C2, C5, and C6.</p>
<p>6,10,14-Trimethyl-2-pentadecanone</p> <p>C₁₈H₃₆O</p> <p>CAS # 502-69-2</p> <p>Log K_{ow}: 6.91 (EPI Suite)</p> <p>Molecular Weight: 268.48</p> <p>Vapor Pressure: 0.000995 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 0.02335 mg/L (EPI Suite)</p>	<p>2-Pentadecanone, 6,10,14-trimethyl-</p> <p>6,10,14-Trimethyl-2-pentadecanone</p> <p>6,10,14-Trimethylpentadecan-2-one</p> <p>Hexahydrofarnesyl acetone</p>	 <p>The structure shows a long saturated hydrocarbon chain with a ketone group at C2 and methyl groups at C6, C10, and C14.</p>

Table 1: Material Identification

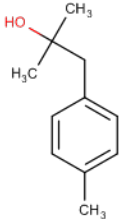
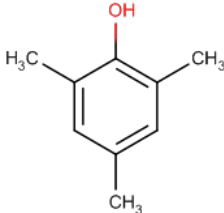
Material	Synonyms	Structure
<p>$\alpha,\alpha,4$-Trimethylphenethyl alcohol</p> <p>C₁₁H₁₆O</p> <p>CAS # 20834-59-7</p> <p>Log K_{ow}: 2.99 (EPI Suite)</p> <p>Molecular Weight: 164.24</p> <p>Vapor Pressure: 0.00159 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 597.8 mg/L (EPI Suite)</p>	<p>$\alpha,\alpha,4$-Trimethylphenethyl alcohol</p> <p>2-Methyl-1-(4-methylphenyl)propan-2-ol</p> <p>Benzeneethanol, $\alpha,\alpha,4$-trimethyl-</p> <p>Methyl-<i>p</i> Dimethyl Benzyl Carbinol</p> <p>$\alpha,\alpha,4$-トリメチルベンゼンエタノール</p>	 <p>The structure shows a benzene ring with a methyl group at the para position (4-position). Attached to the ring is a propyl chain where the alpha carbon (the carbon closest to the ring) is substituted with two methyl groups and a hydroxyl group. The hydroxyl group is shown in red.</p>
<p>2,4,6-Trimethylphenol</p> <p>C₉H₁₂O</p> <p>CAS # 527-60-6</p> <p>Log K_{ow}: 3.15 (EPI Suite)</p> <p>Molecular Weight: 136.19</p> <p>Vapor Pressure: 0.0115 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 1539 mg/L (EPI Suite)</p>	<p>1-Hydroxy-2,4,6-trimethylbenzene</p> <p>1,3,5-Trimethylphenol</p> <p>2-Hydroxymesitylene</p> <p>2,4,6-Trimethylphenol</p> <p>Hydroxymesitylene</p> <p>Mesitol</p> <p>Mesityl alcohol</p> <p>Phenol, 2,4,6-trimethyl-</p>	 <p>The structure shows a benzene ring with a hydroxyl group (OH) at the 1-position and three methyl groups (CH₃) at the 2, 4, and 6 positions. The hydroxyl group is shown in red.</p>


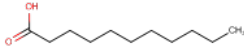
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Undecanenitrile</p> <p>$C_{11}H_{21}N$</p> <p>CAS # 2244-07-7</p> <p>Log K_{ow}: 4.27 (EPI Suite)</p> <p>Molecular Weight: 167.29</p> <p>Vapor Pressure: 0.0146 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 7.695 mg/L (EPI Suite)</p>	<p>Undecanenitrile</p>	
<p>Undecanoic acid</p> <p>$C_{11}H_{22}O_2$</p> <p>CAS # 112-37-8</p> <p>Log K_{ow}: 4.51 (EPI Suite)</p> <p>Molecular Weight: 186.3</p> <p>Vapor Pressure: 0.00291 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 21.39 mg/L (EPI Suite)</p>	<p><i>n</i>-Undecoic acid</p> <p><i>n</i>-Undecylic acid</p> <p>Hendecanoic acid</p> <p>Undecanoic acid</p>	

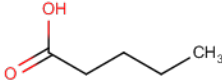
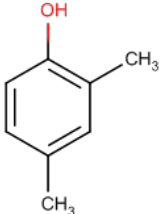
Table 1: Material Identification		
Material	Synonyms	Structure
<p>Valeric acid</p> <p>C₅H₁₀O₂</p> <p>CAS # 109-52-4</p> <p>Log K_{ow}: 1.56 (EPI Suite)</p> <p>Molecular Weight: 102.13</p> <p>Vapor Pressure: 0.495 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 18600 mg/L (EPI Suite)</p>	<p>Pentanoic acid</p> <p>Propylacetic acid</p> <p>Valerianic acid</p> <p>Valeric acid</p> <p>アルカン酸(C=4~30)</p>	
<p>2,4-Xylenol</p> <p>C₈H₁₀O</p> <p>CAS # 105-67-9</p> <p>Log K_{ow}: 2.61 (EPI Suite)</p> <p>Molecular Weight: 122.16</p> <p>Vapor Pressure: 0.067 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 4068 mg/L (EPI Suite)</p>	<p>1-Hydroxy-2,4-dimethylbenzene</p> <p>2,4-Dimethylphenol</p> <p>2,4-Xylenol</p> <p>Phenol, 2,4-dimethyl-</p>	

Table 1: Material Identification		
Material	Synonyms	Structure
<p>2,5-Xylenol</p> <p>C₈H₁₀O</p> <p>CAS # 95-87-4</p> <p>Log K_{ow}: 2.61 (EPI Suite)</p> <p>Molecular Weight: 122.16</p> <p>Vapor Pressure: 0.018 mm Hg @ 20°C (EPI Suite v4.0)</p> <p>Water Solubility: 3835 mg/L (EPI Suite)</p>	<p>1-Hydroxy-2,5-dimethylbenzene</p> <p>2,5-Dimethylphenol</p> <p>2,5-Xylenol</p> <p>Phenol, 2,5-dimethyl-</p>	