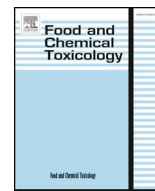




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Short Review

RIFM fragrance ingredient safety assessment, methyl thiobutyrates, CAS Registry Number 2432-51-1



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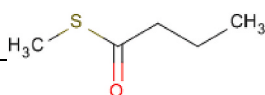
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Version: 012320. This version replaces any previous versions.

Name: Methyl thiobutyrates
CAS Registry Number: 2432-51-1

**Abbreviation/Definition List:**

2-Box Model - A RIFM, Inc. proprietary *in silico* tool used to calculate fragrance air exposure concentration
AF - Assessment Factor
BCF - Bioconcentration Factor
Crema RIFM Model - The Crema RIFM Model uses probabilistic (Monte Carlo) simulations to allow full distributions of data sets, providing a more realistic estimate of aggregate exposure to individuals across a population (Comiskey et al., 2015, 2017; Safford et al., 2015a, 2017) compared to a deterministic aggregate approach
DEREK - Derek Nexus is an *in silico* tool used to identify structural alerts
DRF - Dose Range Finding
DST - Dermal Sensitization Threshold
ECHA - European Chemicals Agency

EU - Europe/European Union
GLP - Good Laboratory Practice
IFRA - The International Fragrance Association
LOEL - Lowest Observable Effect Level
MOE - Margin of Exposure
MPPD - Multiple-Path Particle Dosimetry. An *in silico* model for inhaled vapors used to simulate fragrance lung deposition
NA - North America
NESIL - No Expected Sensitization Induction Level
NOAEC - No Observed Adverse Effect Concentration
NOAEL - No Observed Adverse Effect Level
NOEC - No Observed Effect Concentration
NOEL - No Observed Effect Level
OECD - Organisation for Economic Co-operation and Development
OECD TG - Organisation for Economic Co-operation and Development Testing Guidelines
PBT - Persistent, Bioaccumulative, and Toxic
PEC/PNEC - Predicted Environmental Concentration/Predicted No Effect Concentration
QRA - Quantitative Risk Assessment
REACH - Registration, Evaluation, Authorisation, and Restriction of Chemicals

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<https://doi.org/10.1016/j.fct.2020.111527>

Received 30 January 2020; Received in revised form 11 May 2020; Accepted 11 June 2020

Available online 06 July 2020

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RfD - Reference Dose
 RIFM - Research Institute for Fragrance Materials
 RQ - Risk Quotient
Statistically Significant - Statistically significant difference in reported results as compared to controls with a $p < 0.05$ using appropriate statistical test
 TTC - Threshold of Toxicological Concern
 UV/Vis spectra - Ultraviolet/Visible spectra
 VCF - Volatile Compounds in Food
 VoU - Volume of Use vPvB - (very) Persistent, (very) Bioaccumulative
 WoE - Weight of Evidence

• Revised PEC/PNECs (2015 IFRA VoU): North America and Europe: not applicable; cleared at screening-level

The Expert Panel for Fragrance Safety* concludes that this material is safe as described in this safety assessment

This safety assessment is based on the RIFM Criteria Document (Api, 2015), which should be referred to for clarifications.

Each endpoint discussed in this safety assessment includes the relevant data that were available at the time of writing (version number in the top box is indicative of the date of approval based on a 2-digit month/day/year), both in the RIFM Database (consisting of publicly available and proprietary data) and through publicly available information sources (e.g., SciFinder and PubMed). Studies selected for this safety assessment were based on appropriate test criteria, such as acceptable guidelines, sample size, study duration, route of exposure, relevant animal species, most relevant testing endpoints, etc. A key study for each endpoint was selected based on the most conservative endpoint value (e.g., PNEC, NOAEL, LOEL, and NESIL).

*The Expert Panel for Fragrance Safety is an independent body that selects its own members and establishes its own operating procedures. The Expert Panel is comprised of internationally known scientists that provide RIFM with guidance relevant to human health and environmental protection.

Summary: The existing information supports the use of this material as described in this safety assessment.

Methyl thiobutyrate was evaluated for genotoxicity, repeated dose toxicity, reproductive toxicity, local respiratory toxicity, phototoxicity/photoallergenicity, skin sensitization, and environmental safety. Data show that methyl thiobutyrate is not genotoxic. The repeated dose, reproductive, and local respiratory toxicity endpoints were evaluated using the threshold for toxicological concern (TTC) for a Cramer Class I material, and the exposure to methyl thiobutyrate is below the TTC (0.03 mg/kg/day, 0.03 mg/kg/day, and 1.4 mg/day, respectively). The skin sensitization endpoint was completed using the dermal sensitization threshold (DST) for non-reactive materials (900 $\mu\text{g}/\text{cm}^2$); exposure is below the DST. The phototoxicity/photoallergenicity endpoints were evaluated based on UV spectra; methyl thiobutyrate is not expected to be phototoxic/photoallergenic. The environmental endpoints were evaluated; methyl thiobutyrate was found not to be persistent, bioaccumulative, and toxic (PBT) as per the International Fragrance Association (IFRA) Environmental Standards, and its risk quotients, based on its current volume of use in Europe and North America (i.e., Predicted Environmental Concentration/Predicted No Effect Concentration [PEC/PNEC]), are < 1 .

Human Health Safety Assessment

Genotoxicity: Not genotoxic. (RIFM, 2016a; RIFM, 2016b)

Repeated Dose Toxicity: No NOAEL available. Exposure is below the TTC.

Reproductive Toxicity: No NOAEL available. Exposure is below the TTC.

Skin Sensitization: No safety concerns at current, declared use levels; Exposure is below the DST.

Phototoxicity/Photoallergenicity: Not expected to be phototoxic/photoallergenic. (UV Spectra, RIFM Database)

Local Respiratory Toxicity: No NOAEC available. Exposure is below the TTC.

Environmental Safety Assessment

Hazard Persistence: Screening-level: 2.9 (BIOWIN 3) (EPI Suite v4.11; US EPA, 2012a)

Bioaccumulation: Screening-level: 2.901 L/kg (EPI Suite v4.11; US EPA, 2012a)

Ecotoxicity: Screening-level: Fish LC50: 776.03 mg/L (Salvito (2002))

Conclusion: Not PBT or vPvB as per IFRA Environmental Standards

Risk Assessment:

Screening-level: PEC/PNEC (North America and Europe) < 1 (Salvito (2002))

Critical Ecotoxicity Endpoint: Fish LC50: 776.03 mg/L (Salvito (2002))
RIFM PNEC is: 0.77603 $\mu\text{g}/\text{L}$

1. Identification

- Chemical Name:** Methyl thiobutyrate
- CAS Registry Number:** 2432-51-1
- Synonyms:** Butanethioc acid, S-methyl ester; Methanethiol *n*-butyrate; S-Methyl butanethioate; Methyl thiobutyrate
- Molecular Formula:** $\text{C}_5\text{H}_{10}\text{OS}$
- Molecular Weight:** 118.19
- RIFM Number:** 6739
- Stereochemistry:** Isomer not specified. No stereocenters and no stereoisomers possible.

2. Physical data

- Boiling Point:** 160.71 °C (EPI Suite)
- Flash Point:** 37 °C (GHS), 98 °F; CC (FMA Database)
- Log K_{ow} :** 1.21 (EPI Suite)
- Melting Point:** 31.27 °C (EPI Suite)
- Water Solubility:** 9515 mg/L (EPI Suite)
- Specific Gravity*:** 0.96600 @ 25.00 °C
- Vapor Pressure:** 1.73 mm Hg @ 20 °C (EPI Suite v4.0), 2.6 mm Hg @ 20 °C (FMA Database), 2.43 mm Hg @ 25 °C (EPI Suite)
- UV Spectra:** No significant absorbance between 290 and 700 nm; the molar absorption coefficient is below the benchmark (1000 $\text{L mol}^{-1} \cdot \text{cm}^{-1}$)
- Appearance/Organoleptic*:** A colorless to pale yellow clear liquid with a high sulfurous, cheesy, cabbage, garlic, egg, tomato, tropical fruit, Limburger, metallic odor.

*<http://www.thegoodscentcompany.com/data/rw1035781.html#toorgano>, retrieved on 02/08/18.

3. Volume of use (worldwide band)

- < 0.1 metric ton per year (IFRA, 2015)

4. Exposure

- 95th Percentile Concentration in Hydroalcohols:** 0.00015% (RIFM, 2016c)
- Inhalation Exposure*:** 0.0000058 mg/kg/day or 0.00044 mg/day (RIFM, 2016c)
- Total Systemic Exposure**:** 0.000013 mg/kg/day (RIFM, 2016c)

*95th percentile calculated exposure derived from concentration survey data in the Creme RIFM Aggregate Exposure Model (Comiskey, 2015, 2017; Safford, 2015a, 2017).

**95th percentile calculated exposure; assumes 100% absorption unless modified by dermal absorption data as reported in Section V. It is derived from concentration survey data in the Creme RIFM Aggregate Exposure Model and includes exposure via dermal, oral, and inhalation routes whenever the fragrance ingredient is used in products that include these routes of exposure (Comiskey, 2015, 2017; Safford, 2015a, 2017).

5. Derivation of systemic absorption

- Dermal:** Assumed 100%
- Oral:** Assumed 100%
- Inhalation:** Assumed 100%

6. Computational toxicology evaluation

1. Cramer Classification: Class I, Low* (Expert Judgment)

Expert Judgment	Toxtree v 2.6	OECD QSAR Toolbox v 3.2
I	I	III

*Due to potential discrepancies with the current *in silico* tools (Bhatia et al., 2015), the Cramer Class of the target material was determined using expert judgment based on the Cramer decision tree (Cramer et al., 1978). See the Appendix below for further details.

2. Analogs Selected:

- Genotoxicity: None
- Repeated Dose Toxicity: None
- Reproductive Toxicity: None
- Skin Sensitization: None
- Phototoxicity/Photoallergenicity: None
- Local Respiratory Toxicity: None
- Environmental Toxicity: None

3. Read-across Justification: None

7. Metabolism

Not considered for this risk assessment and therefore not reviewed except where it may pertain in specific endpoint sections as discussed below.

8. Natural occurrence (discrete chemical) or composition (NCS)

Methyl thiobutyrate is reported to occur in the following foods by the VCF*:

- Cheese, various types.
- Fish.
- Hop (*Humulus lupulus*).
- Melon.
- Shrimps (prawn).
- Strawberry (*Fragaria species*).

*Volatile Compounds in Food: Database/Nijssen, L.M.; Ingen-Visscher, C.A. van; Donders, J.J.H. (eds). – Version 15.1 – Zeist (The Netherlands): TNO Triskelion, 1963–2014. A continually updated database containing information on published volatile compounds that have been found in natural (processed) food products. Includes FEMA GRAS and EU-Flavis data.

9. Reach Dossier

Pre-registered for 2010; no dossier available as of 01/23/20.

10. Conclusion

The existing information supports the use of this material as described in this safety assessment.

11. Summary

11.1. Human health endpoint summaries

11.1.1. Genotoxicity

Based on the current existing data and use levels, methyl thiobutyrate does not present a concern for genetic toxicity.

11.1.1.1. Risk assessment. Methyl thiobutyrate was assessed in the BlueScreen assay and found negative for both cytotoxicity

(positive: < 80% relative cell density) and genotoxicity, with and without metabolic activation (RIFM, 2013). BlueScreen is a human cell-based assay for measuring the genotoxicity and cytotoxicity of chemical compounds and mixtures. Additional assays were considered to fully assess the potential mutagenic or clastogenic effects of the target material.

The mutagenic activity of methyl thiobutyrate has been evaluated in a bacterial reverse mutation assay conducted in compliance with GLP regulations and in accordance with OECD TG 471 using the standard plate incorporation method. *Salmonella typhimurium* strains TA98, TA100, TA1535, TA1537, and *Escherichia coli* strain WP2uvrA were treated with methyl thiobutyrate (purity: 99.9%) in dimethyl sulfoxide (DMSO) at concentrations up to 5000 µg/plate. No increases in the mean number of revertant colonies were observed at any tested concentration in the presence or absence of S9 (RIFM, 2016b). Under the conditions of the study, methyl thiobutyrate was not mutagenic in the Ames test.

The clastogenic activity of methyl thiobutyrate was evaluated in an *in vitro* micronucleus test conducted in compliance with GLP regulations and in accordance with OECD TG 487. Human peripheral blood lymphocytes were treated with methyl thiobutyrate (purity: 99.9%) in DMSO at concentrations up to 1180 µg/mL in the presence and absence of S9 for 4 h and in the absence of S9 for 24 h. Methyl thiobutyrate did not induce binucleated cells with micronuclei when tested up to cytotoxic levels concentration in either the presence or absence of an S9 activation system (RIFM, 2016a). Under the conditions of the study, methyl thiobutyrate was considered to be non-clastogenic in the *in vitro* micronucleus test.

Based on the data available, methyl thiobutyrate does not present a concern for genotoxic potential.

Additional References: None.

Literature Search and Risk Assessment Completed On: 01/21/18.

11.1.2. Repeated dose toxicity

There are insufficient repeated dose toxicity data on methyl thiobutyrate or on any read-across materials. The total systemic exposure to methyl thiobutyrate is below the TTC for the repeated dose toxicity endpoint of a Cramer Class I material at the current level of use.

11.1.2.1. Risk assessment. There are no repeated dose toxicity data on methyl thiobutyrate or on any read-across materials that can be used to support the repeated dose toxicity endpoint. The total systemic exposure to methyl thiobutyrate (0.013 µg/kg bw/day) is below the TTC (30 µg/kg bw/day; Kroes, 2007) for the repeated dose toxicity endpoint of a Cramer Class I material at the current level of use.

Additional References: None.

Literature Search and Risk Assessment Completed On: 01/24/18.

11.1.3. Reproductive toxicity

There are insufficient reproductive toxicity data on methyl thiobutyrate or on any read-across materials. The total systemic exposure to methyl thiobutyrate is below the TTC for the reproductive toxicity endpoint of a Cramer Class I material at the current level of use.

11.1.3.1. Risk assessment. There are no reproductive toxicity data on methyl thiobutyrate or on any read-across materials that can be used to support the reproductive toxicity endpoint. The total systemic exposure to methyl thiobutyrate (0.013 µg/kg bw/day) is below the TTC (30 µg/kg bw/day; Kroes, 2007; Laferriere, 2012) for the reproductive toxicity endpoint of a Cramer Class I material at the current level of use.

Additional References: None.

Literature Search and Risk Assessment Completed On: 01/24/18.

Table 1

Maximum acceptable concentrations for methyl thiobutyrate that present no appreciable risk for skin sensitization based on non-reactive DST.

IFRA Category ^a	Description of Product Type	Maximum Acceptable Concentrations in Finished Products Based on Non-reactive DST	Reported 95th Percentile Use Concentrations in Finished Products
1	Products applied to the lips	0.069%	NRU ^b
2	Products applied to the axillae	0.021%	$2.5 \times 10^{-4}\%$
3	Products applied to the face using fingertips	0.41%	$1.0 \times 10^{-5}\%$
4	Fine fragrance products	0.39%	$1.0 \times 10^{-5}\%$
5	Products applied to the face and body using the hands (palms), primarily leave-on	0.10%	0.060%
6	Products with oral and lip exposure	0.23%	$1.7 \times 10^{-4}\%$
7	Products applied to the hair with some hand contact	0.79%	$6.0 \times 10^{-6}\%$
8	Products with significant ano-genital exposure	0.041%	No Data ^c
9	Products with body and hand exposure, primarily rinse-off	0.75%	$6.0 \times 10^{-5}\%$
10	Household care products with mostly hand contact	2.7%	$2.7 \times 10^{-4}\%$
11	Products with intended skin contact but minimal transfer of fragrance to skin from inert substrate	1.5%	No Data ^c
12	Products not intended for direct skin contact, minimal or insignificant transfer to skin	Not Restricted	0.020%

^a For a description of the categories, refer to the IFRA/RIFM Information Booklet.

^b No reported use.

^c Fragrance exposure from these products is very low. These products are not currently in the Creme RIFM Aggregate Exposure Model.

11.1.4. Skin sensitization

Based on the application of the DST, methyl thiobutyrate does not present a safety concern for skin sensitization under the current, declared levels of use.

11.1.4.1. Risk assessment. The chemical structure of this material indicates that it would not be expected to react with skin proteins (Toxtree 2.6.13; OECD Toolbox v4.1). No predictive skin sensitization studies are available for methyl thiobutyrate.

Acting conservatively due to the lack of data, the reported exposure was benchmarked utilizing the non-reactive DST of 900 $\mu\text{g}/\text{cm}^2$ (Safford, 2008, 2011, 2015b; Roberts, 2015). The current exposure from the 95th percentile concentration is below the DST for non-reactive materials when evaluated in all QRA categories. Table 1 provides the maximum acceptable concentrations for methyl thiobutyrate that present no appreciable risk for skin sensitization based on the non-reactive DST. These levels represent maximum acceptable concentrations based on the DST approach. However, additional studies may show it could be used at higher levels.

Additional References: None.

Literature Search and Risk Assessment Completed On: 01/18/18.

11.1.5. Phototoxicity/photoallergenicity

Based on the available UV/Vis spectra, methyl thiobutyrate would not be expected to present a concern for phototoxicity or photoallergenicity.

11.1.5.1. Risk assessment. There are no phototoxicity studies available for methyl thiobutyrate in experimental models. UV/Vis absorption spectra indicate no significant absorption between 290 and 700 nm (RIFM, 2014). The corresponding molar absorption coefficient is well below the benchmark of concern for phototoxicity and photoallergenicity (Henry, 2009). Based on the lack of absorbance, methyl thiobutyrate does not present a concern for phototoxicity or photoallergenicity.

11.1.5.2. UV spectra analysis. UV/Vis absorption spectra (OECD TG 101) were obtained. The spectra indicate no significant absorbance in the range of 290–700 nm. The molar absorption coefficient is below the benchmark of concern for phototoxic effects, 1000 $\text{L mol}^{-1} \cdot \text{cm}^{-1}$ (Henry, 2009).

Additional References: None.

Literature Search and Risk Assessment Completed On: 12/06/

17.

11.1.6. Local Respiratory Toxicity

The MOE could not be calculated due to a lack of appropriate data. The exposure level for methyl thiobutyrate is below the Cramer Class I TTC value for inhalation exposure local effects.

11.1.6.1. Risk assessment. There are no inhalation data available on methyl thiobutyrate. Based on the Creme RIFM Model, the inhalation exposure is 0.00044 mg/day. This exposure is 3182 times lower than the Cramer Class I TTC value of 1.4 mg/day (based on human lung weight of 650 g; Carthew, 2009); therefore, the exposure at the current level of use is deemed safe.

Additional References: None.

Literature Search and Risk Assessment Completed On: 01/27/18.

11.2. Environmental endpoint summary

11.2.1. Screening-level assessment

A screening-level risk assessment of methyl thiobutyrate was performed following the RIFM Environmental Framework (Salvito, 2002), which provides 3 tiered levels of screening for aquatic risk. In Tier 1, only the material's regional VoU, its log K_{OW} , and its molecular weight are needed to estimate a conservative risk quotient (RQ), expressed as the ratio Predicted Environmental Concentration/Predicted No Effect Concentration (PEC/PNEC). A general QSAR with a high uncertainty factor applied is used to predict fish toxicity, as discussed in Salvito et al. (2002). In Tier 2, the RQ is refined by applying a lower uncertainty factor to the PNEC using the ECOSAR model (US EPA, 2012b), which provides chemical class-specific ecotoxicity estimates. Finally, if necessary, Tier 3 is conducted using measured biodegradation and ecotoxicity data to refine the RQ, thus allowing for lower PNEC uncertainty factors. The data for calculating the PEC and PNEC for this safety assessment are provided in the table below. For the PEC, the range from the most recent IFRA Volume of Use Survey is reviewed. The PEC is then calculated using the actual regional tonnage, not the extremes of the range. Following the RIFM Environmental Framework, methyl thiobutyrate was identified as a fragrance material with no potential to present a possible risk to the aquatic environment (i.e., its screening-level PEC/PNEC < 1).

A screening-level hazard assessment using EPI Suite v4.11 (US EPA, 2012a) did not identify methyl thiobutyrate as possibly being either persistent or bioaccumulative based on its structure and

physical–chemical properties. This screening-level hazard assessment considers the potential for a material to be persistent *and* bioaccumulative *and* toxic, or very persistent *and* very bioaccumulative as defined in the Criteria Document (Api, 2015). As noted in the Criteria Document, the screening criteria applied are the same as those used in the EU for REACH (ECHA, 2012). For persistence, if the EPI Suite model BIOWIN 3 predicts a value < 2.2 and either BIOWIN 2 or BIOWIN 6 predicts a value < 0.5 , then the material is considered potentially persistent. A material would be considered potentially bioaccumulative if the EPI Suite model BCFBAF predicts a fish BCF ≥ 2000 L/kg. Ecotoxicity is determined in the above screening-level risk assessment. If, based on these model outputs (Step 1), additional assessment is required, a WoE-based review is then performed (Step 2). This review considers available data on the material's physical–chemical properties, environmental fate (e.g., OECD Guideline biodegradation studies or die-away studies), fish bioaccumulation, and higher-tier model outputs (e.g., US EPA's BIOWIN and BCFBAF found in EPI Suite v4.11). Data on persistence and bioaccumulation are reported below and summarized in the Environmental Safety Assessment section prior to Section 1.

11.2.2. Risk assessment

Based on the current Volume of Use (IFRA, 2015), methyl thiobutyrate does not present a risk to the aquatic compartment in the screening-level assessment.

11.2.2.1. Key studies

11.2.2.1.1. *Biodegradation*. No data available.

11.2.2.1.2. *Ecotoxicity*. No data available.

11.2.2.1.3. *Other available data*. Methyl thiobutyrate has been pre-registered for REACH with no additional data at this time.

11.2.3. Risk assessment refinement

Ecotoxicological data and PNEC derivation (all endpoints reported in mg/L; PNECs in $\mu\text{g/L}$).

Endpoints used to calculate PNEC are underlined.

	LC50 (Fish) (mg/L)	EC50 (<i>Daphnia</i>)	EC50 (Algae)	AF	PNEC ($\mu\text{g/L}$)	Chemical Class
RIFM Framework Screening-level (Tier 1)	<u>776.03</u>			1000000	0.77603	

Exposure information and PEC calculation (following RIFM Environmental Framework: Salvito, 2002).

Exposure	Europe (EU)	North America (NA)
Log K_{ow} Used	1.21	1.21
Biodegradation Factor Used	0	0
Dilution Factor	3	3
Regional Volume of Use Tonnage Band	< 1	< 1
Risk Characterization: PEC/PNEC	< 1	< 1

Based on available data, the RQ for this material is < 1 . No further assessment is necessary.

The RIFM PNEC is 0.77603 $\mu\text{g/L}$. The revised PEC/PNECs for EU and NA are not applicable. The material was cleared at the screening-

level; therefore, it does not present a risk to the aquatic environment at the current reported volumes of use (IFRA, 2015).

Literature Search and Risk Assessment Completed On: 01/22/18.

12. Literature Search*

- **RIFM Database:** Target, Fragrance Structure-Activity Group materials, other references, JECFA, CIR, SIDS
- **ECHA:** <https://echa.europa.eu/>
- **NTP:** <https://ntp.niehs.nih.gov/>
- **OECD Toolbox**
- **SciFinder:** <https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf>
- **PubMed:** <https://www.ncbi.nlm.nih.gov/pubmed>
- **National Library of Medicine's Toxicology Information Services:** <https://toxnet.nlm.nih.gov/>
- **IARC:** <https://monographs.iarc.fr>
- **OECD SIDS:** <https://hvpchemicals.oecd.org/ui/Default.aspx>
- **EPA ACToR:** <https://actor.epa.gov/actor/home.xhtml>
- **US EPA HPVIS:** https://ofmpub.epa.gov/opthpv/public_search_publicdetails?submission_id=24959241&ShowComments=Yes&sqlstr=null&recordcount=0&User_title=DetailQuery%20Results&EndPointRpt=Y#submission
- **Japanese NITE:** https://www.nite.go.jp/en/chem/chrip/chrip_search/systemTop
- **Japan Existing Chemical Data Base (JECDB):** http://dra4.nihs.go.jp/mhlw_data/jsp/SearchPageENG.jsp
- **Google:** <https://www.google.com>
- **ChemIDplus:** <https://chem.nlm.nih.gov/chemidplus/>

Search keywords: CAS number and/or material names.

*Information sources outside of RIFM's database are noted as appropriate in the safety assessment. This is not an exhaustive list. The links listed above were active as of 01/23/20.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix

Explanation of Cramer Classification

Due to potential discrepancies with the current *in silico* tools (Bhatia et al., 2015), the Cramer Class of the target material was determined using expert judgment based on the Cramer decision tree (Cramer et al., 1978).

Q1. Normal constituent of the body? No

- Q2. Contains functional groups associated with enhanced toxicity? No
- Q3. Contains elements other than C, H, O, N, and divalent S? No
- Q5. Simply branched aliphatic hydrocarbon or a common carbohydrate? No
- Q6. Benzene derivative with certain substituents? No
- Q7. Heterocyclic? No
- Q16. Common terpene (see Cramer et al., 1978 for detailed explanation)? No
- Q17. Readily hydrolyzed to a common terpene? No
- Q19. Open chain? Yes
- Q20. Aliphatic with some functional groups (see Cramer et al., 1978 for detailed explanation)? Yes
- Q21.3 or more different functional groups? No
- Q18. One of the list (see Cramer et al., 1978 for detailed explanation on list of categories)? No. Class I (Low class)

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