BUTYL MERCAPTAN

CAS number:	109-79-5
Synonyms:	n-Butanethiol, 1-butanethiol, butane-1-thiol
Chemical formula:	C_4H_9SH

Workplace exposure standard (retained)

TWA:	**0.5 ppm (1.8 mg/m^3)**
STEL:	**—**
Peak limitation:	**—**
Notations:	**—**
IDLH:	**500 ppm (1,844 mg/m^3)**
Sampling and analysis:	The recommended value is readily quantifiable through currently available sampling and analysis techniques.

Recommendation and basis for workplace exposure standard

A TWA of 0.5 ppm (1.8 mg/m^3) is recommended to protect for irritation of mucous membranes in exposed workers.

Discussion and conclusions

Butyl mercaptan is typically used as a solvent and an intermediate in pesticide production. It is used as an odourant for natural gas due to its recognisably disagreeable odour at extremely low concentrations (0.0001–0.001 ppm). Ethyl mercaptan is structurally similar, exhibits a comparable toxicological profile and is more thoroughly investigated than the butyl homologue (ACGIH, 2018).

Critical effects of exposure are irritation of mucous membranes and at higher concentrations, central nervous system effects including sweating, nausea, headache and muscular weakness (ACGIH, 2018). A NOAEL of 10 ppm for maternal toxicity is reported in a developmental study with rats exposed to n-butyl mercaptan (six hours per day for 14 days). A NOAEL in mice could not be established for the same concentration ranges due to maternal and developmental toxicity at 10 ppm (HCOTN, 2005).

The recommended TWA of 0.5 ppm (1.8 mg/m^3) is based on a NOAEL of 0.5 ppm for the analogous ethyl mercaptan for mucous membrane irritation and altered taste perception in humans (ACGIH, 2018). This TWA is expected to be sufficiently protective for irritation and reproductive adverse effects.

Recommendation for notations

Not classified as a carcinogen according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS).

Not classified as a skin sensitiser or respiratory sensitiser according to the GHS.

There are insufficient data to recommend a skin notation.

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APPENDIX

Primary sources with reports

Source	Year set	Standard
SWA	***1995***	***TWA: 0.5 ppm (1.8 mg/m^3)***
ACGIH	***2001***	***TLV-TWA: 0.5 ppm (1.8 mg/m^3)***

TLV-TWA intended to minimise potential for irritation to mucous membranes and, at higher concentrations, adverse CNS effects, such as sweating, nausea, vomiting, headache, weakness and malaise.

NOAEL of 0.5 ppm for mucous membrane irritation and altered taste perception with the analogous ethyl mercaptan in humans (3 h/d, 5–10 d) is used to derive the TLV-TWA due to lack of substance-specific exposure data.

Ethyl mercaptan is more thoroughly investigated and has the same critical effects and comparable odour threshold.

Insufficient data to recommend a TLV-STEL or notations for skin, sensitisation or carcinogenicity.

Summary of data:

Human data:

- Accidental release in a laboratory caused exposure of 7 workers at 50–500 ppm for 1 h:
  - all presented muscular weakness, malaise, flushing of the face, increased breathing and dilated pupils
  - 6 presented sweating, nausea, vomiting and headache
  - 3 presented confusion
  - 1 lost consciousness for 20 min
  - 6 of the workers recovered after 1 d.

Animal data:

- LC_{50}: 2,500 ppm (mice, 4 h), 4,020 ppm (rats, 4 h):
  - effects included mucous membrane irritation, increased respiration and CNS depression, e.g. staggering, weakness, partial paralysis, cyanosis and sedation
- Liver and kidney damage caused at near-lethal doses (not specified) in surviving animals *via* oral or *ip* administration, observed up to 20 d post-administration (rats and mice, no further information provided)
- Slight to moderate eye irritation in rabbits (no further information provided)
- No dermal changes at 0.2 mL dose on shaved skin (guinea pigs, 20% solvent and concentration expression not specified, 10 d).

DFG	***2005***	***MAK: 0.5 ppm (1.8 mg/m^3)***

Summary of additional information:

MAK established in 1969 in analogy to the TLV at the time.

No evidence to support sensitising effects.

Metabolic oxidation to disulfides yields ROS as co-products, which may lead to oxidative stress.

Human data:

- Elaboration of human case study presented in ACGIH:
  - clinical and biochemical examinations of exposed workers were in normal ranges 30–40 d post-exposure.

Animal data:

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Source	Year set	Standard
• Blood plasma half-life: 8 d (chickens) • CNS suppression and death by respiratory arrest caused at high doses (not specified) occur irrespective of administration route in rodents • LC_{50}: 4,020–6,060 ppm (rats, 4 h) • LD_{50}: 1,500–1,800 mg/kg (rats, oral) • LD_{50}: 399 mg/kg (rats, *ip*) • $LD_{50:}$ >34,600 mg/kg (rabbits, dermal) • Increased relative organ weights in repeat inhalation dose-ranging chamber study with 200–1,900 ppm exposures (rats, n=20, 6 h/d, 14 d): o 200 ppm; increased kidney weights (and lung and trachea weights only in males) o histological examination of kidneys only carried out on dead animals and control group • NOAEL: 9 ppm for haematological changes in follow-up inhalation study reported (rats, n=30, 6 h/d, 5 d/wk, 13 wk): o LOAEL: 70 ppm, 150 ppm caused slight to moderate fibrosis in lungs o only animals from 150 ppm exposure group were examined histopathologically • NOAEL: 152–200 ppm for developmental effects from separate studies (rats, 6 h/d, 14 d): o 100% foetal resorption at 1,100 ppm • Bacterial and mouse cell *in vitro* mutagenicity studies reported inconclusive evidence of genotoxicity due to unknown substance purity: o non-mutagenic from bacterial experiments o slightly mutagenic from sister chromatid exchange experiment with Chinese hamster ovary cells o inconclusive positive results in mouse lymphoma mutation test due to non-concentration-dependent effects • Neuropathological effects in two repeat oral dose studies with chickens at 50 mg/kg/d (90 d) and 200 mg/kg/d (28 d) • No data available for carcinogenicity.		
SCOEL	***NA***	***NA***
No report.		
OARS/AIHA	***NA***	***NA***
No report.		
HCOTN	***2005***	***8-hour TWA: 0.5 ppm (1.5 mg/m^3)***
Summary of additional data: Available toxicological data insufficient to recommend health-based OEL. Current TWA is considered too high based on maternal and developmental toxicity reported at 10 ppm in mice. Animal data: • LC_{50}: 770 ppm (dogs, 30 min) • LD_{50}: 3,000 mg/kg (mice) • Single oral dose NOAEL: 100 mg/kg for histological and behavioural changes (chickens) • Inhalational NOAEL of 9 ppm for haematological effect in repeat inhalation chamber study with rats cited in DFG, 2005 is not considered a NOAEL due to lack of histopathological examination of the lower exposure groups • No changes in developmental endpoints at 10–152 ppm exposures (rats, 6 h/d, 14 d) (same study cited in DFG, 2005) o NOAEL: 10 ppm for maternal toxicity		

Source	Year set	Standard
		○ a NOAEL could not be established in mice (11 d) due to both maternal (reduced bw gains) and developmental toxicity at 10 ppm (increased incidence of cleft palate, not statistically significant because of high incidence in control group).

Secondary source reports relied upon

Source		Year	Additional information
OECD	✓	2010	Assessed with other butyl mercaptan isomers due to similarities in structure and toxicological/environmental fate.
US NIOSH	✓	1994	IDLH based on acute inhalation toxicity data in workers and animals and to be consistent with ethyl mercaptan.

Carcinogenicity — non-threshold based genotoxic carcinogens

Is the chemical mutagenic? No

The chemical is a non-threshold based genotoxic carcinogen.

Notations

Source	Notations
SWA	—
HCIS	NA
NICNAS	NA
EU Annex	NA
ECHA	NA
ACGIH	—
DFG	—
SCOEL	NA
HCOTN	—
IARC	NA
US NIOSH	NA

NA = not applicable (a recommendation has not been made by this Agency); — = the Agency has assessed available data for this chemical but has not recommended any notations

Skin notation assessment

Calculation
Insufficient data to assign a skin notation.

IDLH

Is there a suitable IDLH value available? Yes

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Additional information

Molecular weight:	90.19
Conversion factors at 25°C and 101.3 kPa:	1 ppm = Number mg/m^3; 1 mg/m^3 = Number ppm
This chemical is used as a pesticide:	✓
This chemical is a biological product:	☐
This chemical is a by-product of a process:	☐
A biological exposure index has been recommended by these agencies:	☐ ACGIH ☐ DFG ☐ SCOEL

Workplace exposure standard history

Year	Standard
Click here to enter year	

References

American Conference of Industrial Hygienists (ACGIH®) (2018) TLVs® and BEIs® with 7th Edition Documentation, CD-ROM, Single User Version. Copyright 2018. Reprinted with permission. See the *TLVs® and BEIs® Guidelines section* on the ACGIH website.

Deutsche Forschungsgemeinschaft (DFG) (2005) Butanethiol – MAK value documentation.

Health Council of the Netherlands (HCOTN) (2005) Butane-1-thiol. Health-based Reassessment of Administrative Occupational Exposure Limits. The Hague: Health Council of the Netherlands; publication no. 2000/15OSH/144.

Organisation for Economic Cooperation and Development (OECD) (2012) SIAM agreed conclusions report – C2-C4 Aliphatic Thiols Category.

US National Institute for Occupational Safety and Health (NIOSH) (1994) Immediately dangerous to life or health concentrations – n-butyl mercaptan.

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