

PHENYL MERCAPTAN

CAS number: 108-98-5

Synonyms: Benzenethiol, thiophenol, phenylthiol, phenylmercaptan, mercaptobenzene

Chemical formula: C₆H₆S

Structural formula: —

Workplace exposure standard (amended)

TWA: 0.1 ppm (0.45 mg/m³)

STEL: —

Peak limitation: —

Notations: Sk.

IDLH: —

Sampling and analysis: The recommended value is quantifiable through available sampling and analysis techniques.

Recommendation and basis for workplace exposure standard

A TWA of 0.1 ppm (0.45 mg/m³) is recommended to protect for irritation and potential liver and kidney damage in exposed workers.

Discussion and conclusions

Phenyl mercaptan is used in the production of polymers, pesticides and pharmaceuticals and as a food additive.

Critical effects of exposure are irritation of the eyes and upper respiratory tract and headaches. In addition, liver and kidney damage is observed in exposed animals (ACGIH, 2018; HCOTN, 2004).

The available toxicological database is limited. Inhalational exposure in humans is associated with eye and upper respiratory tract irritation and headaches after acute exposures at 0.7 ppm (HCOTN, 2004). Phenyl mercaptan is acutely toxic by inhalation in animals with four-hour LC₅₀ values between 28 and 33 ppm in mice and rats, respectively. Systemic liver and kidney damage is observed in a combined feeding developmental study with rats at a LOAEL of 9 mg/kg/day, which is approximately equivalent to an inhalational dose of 10 to 20 ppm in rats (ACGIH, 2018; HCOTN, 2004).

Due to the lack of chronic exposure data for irritation in humans, a TWA of 0.1 ppm by ACGIH (2018) is recommended and is expected to be protective of this endpoint as observed in humans and systemic liver and kidney effects as evidenced in rats. This recommendation is supported by HCOTN (2004) evaluations stating that the administrative TWA of 0.5 ppm is too high but there are insufficient data to set a health-based TWA.

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.

A skin notation is recommended based on evidence suggesting potential dermal absorption and adverse systemic effects in animals.

DRAFT

APPENDIX

Primary sources with reports

Source	Year set	Standard
SWA	1991	TWA: 0.5 ppm (2.3 mg/m³)
ACGIH	2004	TLV-TWA: 0.1 ppm (0.45 mg/m³)
<p>TLV-TWA intended to protect for eye and skin irritation and potential adverse CNS effects. Skin notation recommended based on relatively low dermal LD₅₀ values in rats and rabbits.</p> <p>Summary of information:</p> <p>Toxicological database is limited. TLV-TWA recommended based on weight of evidence from acute inhalation and repeat oral dose data in animals. Oral dose endpoints are converted to inhalational equivalents to support recommendation. Based on LC₅₀ of 30 ppm in rats and liver and kidney effects observed at 9 mg/kg/d \approx 10–20 ppm inhalation dose in rats, TLV-TWA of 0.1 ppm expected to be protective.</p> <p>Human data:</p> <ul style="list-style-type: none"> Can cause severe dermatitis, headaches and dizziness (no further details provided). <p>Animal data:</p> <ul style="list-style-type: none"> LC₅₀: 28 ppm (mice, 4 h), 33 ppm (rats, 4 h) Oral LD₅₀: 46 mg/kg (rats); dermal LD₅₀: 300 mg/kg (rats), 134 mg/kg (rabbits): <ul style="list-style-type: none"> symptoms, regardless of administration route, are hyperpnoea, incoordination, weakness, paralysis, cyanosis, respiratory depression and coma which leads to death Lung, liver and kidney damage at 31–79 ppm (mice, duration not specified) Severely irritating to eyes and skin (rabbits, no further details provided) Adrenal and kidney damage reported at 3.5 mg/kg in repeat ip injection study (species not identified, 9 doses over 3 wk) Foetal mortality and congenital malformations at 50 mg/kg/d in developmental gavage study (rats, rabbits, duration not specified, administered during gestation): <ul style="list-style-type: none"> foetal developmental NOAEL: 20 mg/kg/d (rats), 40 mg/kg/d (rabbits) NOAEL converted to 8 h inhalational equivalents: 24 ppm (rats), 10 ppm (rabbits) Dose-dependent liver and kidney effects (not specified) at 9–35 mg/kg/d in multigeneration repeat gavage study (rats, 16 wk F₀ and 81 d F₁); reduced sperm motility and inhibited sperm production at 18–35 mg/kg/d: <ul style="list-style-type: none"> not considered reproductively toxic due to adverse liver and kidney effects being more sensitive endpoints offspring body weight generally inconsistent with dose, most pronounced effects at 35 mg/kg/d \approx 40 ppm over 8 h (rats) Non-mutagenic <i>in vitro</i> with bacteria, low survival at 25 μg/plate with <i>S. typhimurium</i> TA100 strain. <p>Insufficient data to recommend a TLV-STEL or notations for carcinogenicity or sensitisation.</p>		
DFG	NA	NA
No report.		

Source	Year set	Standard
SCOEL	NA	NA
No report.		
OARS/AIHA	NA	NA
No report.		
HCOTN	2004	TWA: 0.5 ppm (2 mg/m³)
<p>Summary of additional information:</p> <p>Current administrative OEL considered too high based on the available evidence. However, recommendation of a HBROEL is not possible due to insufficient quantitative data on irritation endpoints in humans, which are limited to a poorly documented volunteer study.</p> <p>Derivation from a systemic NOAEL of 9 mg/kg/d for liver and kidney toxicity reported in a developmental study with rats (also cited in ACGIH, 2018) would result in an equivalent inhalational concentration of 0.1 ppm (0.5 mg/m³) following conversion to an inhalational dose and application of uncertainty factors:</p> <ul style="list-style-type: none"> UF of 7/5 and 1/4 applied to account for exposure duration in the study and allometric scaling from rats to humans, respectively. An overall UF of 36 to account for the absence of a NOAEL and inter and intraspecies differences, results in 0.0875 mg/kg or 0.5 mg/m³ as a potential HBROEL assuming a respiratory volume of 10 m³ in a 70 kg individual during an 8 h shift. <p>Human data:</p> <ul style="list-style-type: none"> One inhalation (not specified) at 0.7 ppm caused headache and eye, nose and throat irritation in volunteer study (n=6); eye irritation persisted for several hours (not specified) Methaemoglobin formation shown <i>in vitro</i> in human red blood cells, classified as a haemolytic agent. <p>Animal data:</p> <ul style="list-style-type: none"> Signs of irritation, ocular oedema, erythema, nasal discharge at 242–590 ppm (rats, 1 h) LC₅₀: 418 (rats, 1 h); lung haemorrhage observed in necropsy Agency notes discrepancy between rat LD₅₀ of 46 mg/kg and repeat oral doses in developmental study at 50 mg/kg/d (also cited in ACGIH, 2018) Lung haemorrhage, discoloured livers and kidneys and signs of intestinal irritation at ≈85 ppm in repeat inhalation study (mice, 6–8 h/d, 4 d, also cited in ACGIH, 2018) Non-mutagenic <i>in vitro</i> in bacteria, no <i>in vivo</i> studies available for assessment. 		

Secondary source reports relied upon

Source	Year	Additional information
ECHA	* 2019	Only reproductive/developmental studies presented. No additional information.

Carcinogenicity — non-threshold based genotoxic carcinogens

Is the chemical mutagenic? Insufficient data

Is the chemical carcinogenic with a mutagenic mechanism of action? Insufficient data

Insufficient data are available to determine if the chemical is a non-threshold based genotoxic carcinogen.

Notations

Source	Notations
SWA	—
HCIS	NA
NICNAS	NA
EU Annex	NA
ECHA	NA
ACGIH	Skin
DFG	NA
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	
Adverse effects in human case study:	yes
Dermal LD ₅₀ ≤ 1000 mg/kg:	yes
Dermal repeat-dose NOAEL ≤ 200 mg/kg:	
Dermal LD ₅₀ /Inhalation LD ₅₀ < 10:	no
<i>In vivo</i> dermal absorption rate > 10%:	
Estimated dermal exposure at WES > 10%:	
a skin notation is not warranted	

IDLH

Is there a suitable IDLH value available? No

Additional information

Molecular weight:	110.18
Conversion factors at 25°C and 101.3 kPa:	1 ppm = 4.5 mg/m ³ ; 1 mg/m ³ = 0.22 ppm
This chemical is used as a pesticide:	<input checked="" type="checkbox"/>
This chemical is a biological product:	<input type="checkbox"/>
This chemical is a by-product of a process:	<input type="checkbox"/>
A biological exposure index has been recommended by these agencies:	<input type="checkbox"/> ACGIH <input type="checkbox"/> DFG <input type="checkbox"/> 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.

Health Council of the Netherlands (HCOTN) (2004) Benzenethiol. Health-based Reassessment of Administrative Occupational Exposure Limits. The Hague: Health Council of the Netherlands; publication no. 2000/15OSH/095.