

OCTANE

CAS number: 111-65-9

Synonyms: Normal octane, octane, alkane C(8)

Chemical formula: C₈H₁₈

Structural formula: —

Workplace exposure standard (retained)

TWA: 300 ppm (1,400 mg/m³)

STEL: 375 ppm (1,750 mg/m³)

Peak limitation: —

Notations: —

IDLH: 1,000 ppm

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

Recommendation and basis for workplace exposure standard

A TWA of 300 ppm (1,400 mg/m³) is recommended to protect for narcosis and respiratory irritation in exposed workers.

A STEL of 375 ppm (1,750 mg/m³) is recommended to protect for central nervous system depression in acutely exposed workers.

Discussion and conclusions

Octane is used as a solvent and additive in distillations. It is also present in petrol as an isomeric mixture.

Critical effects of exposure include mucous membrane irritation and narcosis (DFG, 2014); however, cases of human exposure are poorly documented.

Substance-specific animal exposure data are limited to acute inhalation studies. In these acute studies, signs of central nervous system (CNS) depression are observed at 1,000 ppm in rats with a NOAEC of 500 ppm (DFG, 2017) and respiratory tract irritation is reported above 11,700 ppm in mice (ACGIH, 2018). A NOAEC of 590 ppm and LOAEC of 1,600 ppm for CNS depression for *n*-heptane (structurally and toxicologically related to octane) are reported in a sub-chronic inhalation study in rats (ACGIH, 2018; DFG, 2014). Kidney and liver effects observed in rodents are not considered relevant to human exposure due to species-specific metabolism (DFG, 2017).

Based on these animal exposure data, the TWA of 300 ppm derived by ACGIH (2018) is recommended to be retained and is expected to protect for narcosis and mucous membrane irritation in exposed workers. The recommended STEL of 375 ppm is expected to protect for potential acute CNS depression as observed in rats above 1,000 ppm.

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	1991	TWA: 300 ppm (1,400 mg/m³); STEL: 375 ppm (1,750 mg/m³)
ACGIH	2001	TLV-TWA: 300 ppm (1,401 mg/m³)
<p>TLV-TWA recommended for all octane isomers and intended to protect for irritation of mucous membranes and narcosis at higher concentrations. Peak exposures near the TLV-TWA should be controlled to 10% LEL of 1,000 ppm due to high flammability.</p> <p>TLV-STEL of 375 ppm withdrawn in 1999.</p> <p>Summary of data:</p> <p>In the absence of robust toxicological data, median respiratory depression (RD₅₀) used as line of evidence to derive TLV-TWA from established ratio of $0.03 \times \text{RD}_{50} \approx \text{TLV} \approx 540 \text{ ppm}$, which supports analogy to other alkanes. Neurotoxicity not expected at TLV-TWA due to low potential for formation of neurotoxic diketone metabolites.</p> <p>Human data:</p> <ul style="list-style-type: none"> Narcotic at 8,000–10,000 ppm; fatal at 13,500 ppm (no further details provided): <ul style="list-style-type: none"> data suggest octane is as potent or twice as potent as heptane <p>Animal data:</p> <ul style="list-style-type: none"> Sensitivity of mucous membrane irritation and narcosis endpoints increases with molecular weight (species and experimental details not specified) Narcosis at 6,660–13,700 ppm (mice, 30–90 min): <ul style="list-style-type: none"> respiratory arrest occurred at 16,000 ppm in 1/4 mice (<5 min) or at 32,000 ppm in 4/4 mice (<3 min) RD₅₀: 18,150 ppm (mice, duration not specified); extrapolated from experimental data, highest tested dose of 11,700 ppm had no effect (as cited in DFG, 2014). <p>Insufficient data to recommend a TLV-STEL and notations for carcinogenicity, skin absorption and sensitisation.</p>		
DFG	1961 Octane isomers except trimethylpentanes	MAK: 500 ppm (2,370 mg/m³)
	2016 Trimethylpentanes	MAK: 100 ppm (470 mg/m³)
<p>Summary of additional data:</p> <p>Critical effects are mucous membrane irritation and CNS depression. In the absence of robust repeat exposure data, MAK evaluated for all octane isomers except trimethylpentane (isooctane) and based on acute octane exposure data and analogy to <i>n</i>-heptane and <i>n</i>-nonane. Irritant effects are produced at 2,000 ppm of <i>n</i>-octane in acutely exposed rats and a NOEC of 590 ppm of <i>n</i>-heptane for signs of CNS depression with a corresponding LOEC of 1,600 ppm is reported in a sub-chronic inhalation study in rats.</p> <p>Trimethylpentane evaluated separately due to species and sex-specific nephrotoxicity and historical carcinogenicity notation. Trimethylpentane MAK derived from NOAEC of 500 ppm in rat acute exposure study and extrapolated to an 8-h shift assuming a half-life of 1 h calculated from PBPK modelling. No reliable sub-chronic exposure data available.</p>		

Source	Year set	Standard
<p>Human data:</p> <ul style="list-style-type: none"> 20% pulmonary retention expected based on values for <i>n</i>-hexane and <i>n</i>-heptane Inhalation caused respiratory tract irritation, respiratory depression, pulmonary oedema, and excitation of the CNS (no further details provided) Peripheral neuropathy associated with <i>n</i>-hexane exposure not observed for <i>n</i>-octane. <p>Animal data:</p> <p><i>Trimethylpentane</i></p> <ul style="list-style-type: none"> RD₅₀ for trimethylpentane >1,000 ppm (mice, 30 min) NOAEC for slight neurotoxicity: 500 ppm of trimethylpentane reported in acute inhalation study (rats, 60 min); LOAEC: 1,000 ppm. <p><i>Octane isomers except trimethylpentane</i></p> <ul style="list-style-type: none"> LC₅₀: 24,895 ppm (rats, 4 h) RD₅₀: 18,200 ppm (mice, 10 min, calculated); RD₅₀ for <i>n</i>-heptane: 15,600 ppm (10 min), 17,400 ppm (30 min) Dermal penetration <i>in vitro</i> (rat skin): 0.56 ng/cm²/h Inhaled doses distributed in body; accumulation in adipose tissue Nephropathy from oral doses of various octane isomers except <i>n</i>-octane in rats Slight to moderate kidney damage with isomeric mixture at 800 mg/kg compared to controls in repeat gavage dose study (rats, 14 d) OECD-compliant sub-chronic inhalation study reported NOAEC at highest tested dose of 1,600 ppm of <i>n</i>-octane (rats, 13 wk, exposure frequency not specified in document) No kidney damage with pure <i>n</i>-octane at 1,400 mg/kg every 2 d as oral dose (rats, 14 d) Measures of cell proliferation not changed by incubation of Syrian hamster embryo cells with <i>n</i>-octane or 2-methylheptane Chronic inhalation study using unleaded petrol that contained octane isomer mixtures at ≈17% caused sex and species-specific liver and kidney tumours; exposure groups 0, 67, 292, and 2,056 ppm (rats, mice, 2 yr): <ul style="list-style-type: none"> kidney tumours observed in male rats at 67 ppm (none in controls) liver tumours observed in female mice in all exposure groups, slightly higher than controls at 67 ppm No genotoxicity data provided. <p>Carcinogenicity notation not recommended due to insufficient data. Skin notation not warranted based on low dermal penetration rate <i>in vitro</i>. Sensitiser notation not warranted based on lack of evidence in cases of human exposure.</p>		
SCOEL	NA	NA
No report.		
OARS/AIHA	NA	NA
No report.		
HCOTN	2005	TWA: 300 ppm (1,450 mg/m³)
<p>Summary of additional data:</p> <p>Insufficient data to comment on the suitability of the current administrative OEL.</p> <p>Human data:</p>		



Source	Year set	Standard
<ul style="list-style-type: none"> Erythema, hyperaemia, itching sensation, and inflammation when applied to forearm (1 h) or thigh (5 h) in volunteer dermal application study. <p>Animal data:</p> <ul style="list-style-type: none"> No significant changes in motor activity and behaviour at 2,940 ppm (rats, 8 h/d, 3 d) Cumulative inhalational exposure at 3,000, 5,600 and 7,000 ppm caused delayed behavioural responses in rats exposed at 40 min intervals over 4 h; NOAEC: 1,000 ppm. 		

Secondary source reports relied upon

Source	Year	Additional information
ECHA	✓ 2019	<ul style="list-style-type: none"> Long-term inhalational DNEL: 430 ppm based on repeat dose systemic NOAEC in animals; neither study presented this NOAEC nor is the derivation of the DNEL discussed.
OECD	* 2010	<ul style="list-style-type: none"> Not suitable. Grouped with C7-C9 hydrocarbons.
US NIOSH	✓ 1994	<ul style="list-style-type: none"> IDLH of 1,000 ppm based strictly on 10% of LEL.

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	—
NICNAS	NA
EU Annex	—
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, based on LEL

Additional information

Molecular weight:	114.22
Conversion factors at 25°C and 101.3 kPa:	1 ppm = 4.74 mg/m ³ ; 1 mg/m ³ = 0.211 ppm
This chemical is used as a pesticide:	<input 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.

Deutsche Forschungsgemeinschaft (DFG) (2004) Octane and its Isomers (except trimethylpentane isomers) – MAK value documentation.

Deutsche Forschungsgemeinschaft (DFG) (2017) Trimethylpentane (all isomers) – MAK value documentation.

European Chemicals Agency Regulation (ECHA) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH).

Health Council of the Netherlands (HCOTN) (2005) Octane. Health-based Reassessment of Administrative Occupational Exposure Limits. The Hague: Health Council of the Netherlands; publication no. 2000/15OSH/156.

Organisation for Economic Cooperation and Development (OECD) (2010) SIDS initial assessment profile – Octane.

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

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