

DICYCLOPENTADIENYL IRON

CAS number: 102-54-5

Synonyms: Ferrocene

Chemical formula: C₁₀H₁₀Fe

Workplace exposure standard (amended)

TWA: 0.1 mg/m³

STEL: —

Peak limitation: —

Notations: —

IDLH: —

Sampling and analysis: There is uncertainty regarding quantification of the recommended value with available sampling and/or analysis techniques.

Recommendation and basis for workplace exposure standard

A TWA of 0.1 mg/m³ is recommended to protect for irritation of the upper respiratory tract and bioaccumulation of iron in exposed workers.

Discussion and conclusions

Dicyclopentadienyl iron is used as anti-knock agent and combustion catalyst.

Limited exposure data exist. From animal toxicity data, critical effects of exposure are irritation to the upper respiratory tract and, at higher concentrations, bioaccumulation of iron, particularly in the liver.

The recommended TWA of 0.1 mg/m³ is based on a LOAEC of 3.0 mg/m³ for the formation of lesions in the nasal epithelia of mice and rats in a 13 week inhalation study reported by HCOTN (2002). This is absent from the ACGIH (2018) assessment. The TWA was derived by dividing the LOAEC by a 24-fold (3 x 8) uncertainty factor to account for the absence of NOAEL, intra- and interspecies variation and differences between experimental exposures and workplace conditions; and rounding down the results.

Carcinogenic activity, dermal absorption, and sensitisation potential were not evaluated in the available assessments (ACGIH, 2018; HCOTN, 2002) or other available source documentation due to a lack of data. A detailed review of these properties should be prioritised in subsequent reviews.

Recommendation for notations

Not classified as a carcinogen according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). However, a review of the carcinogenicity notation is recommended as notation source data were found to be inadequate for this evaluation.

Not classified as a skin or respiratory sensitiser according to the GHS. However, a review of the sensitiser notation is recommended as notation source data were inadequate for this evaluation.

There are insufficient data to recommend a skin notation.

APPENDIX

Primary sources with reports

Source	Year set	Standard
SWA	1991	TWA: 10 mg/m³
ACGIH	2001	TWA: 10 mg/m³
<p>TLV-TWA intended to minimise potential for excessive bioaccumulation of iron, particularly in the liver.</p> <p>Summary of data:</p> <p>Toxicological data are extremely limited and no human exposure data are reported. However, the substance is considered to have relatively low toxicity based on the available animal data and absence of reported effects in exposed workers. When used as an anti-knocking agent, the resulting combustion product is iron oxide. TLV-TWA derivation not discussed.</p> <p>Human data:</p> <ul style="list-style-type: none"> • None presented. <p>Animal data:</p> <ul style="list-style-type: none"> • LD₅₀: 832 mg/kg (mice, oral) • May be used as a hematinic in animals • Intracellular accumulation of iron (haemosiderosis) reported in sub-chronic daily feeding study with dogs, treatment range: 30–300 mg/kg/d (6 mo), 1,000 mg/kg/d (3 mo) <ul style="list-style-type: none"> ○ dose-dependent haemosiderosis reported in 1,000 mg/kg group; cirrhosis and liver haemosiderosis in the 300–1,000 mg/kg/d groups ○ testicular hyperplasia noted after 6 mo in 100–300 mg/kg/d groups; no other evidence of latent effects of excess iron ○ uncertain if 30 mg/kg/d group represents a NOAEL • Mutagenic in <i>Drosophila melanogaster</i> recessive lethal test at concentrations that were lethal to 30% of the experimental animals within 24 h (concentration not specified) • Inhalation study with rats showed deposition of the substance in the nasopharynx and lungs (17 min exposure) <ul style="list-style-type: none"> ○ respiratory retention lasted several weeks (not specified) ○ clearance half-time of 200 d in the bronchopulmonary region, 70 d in nasopharynx. <p>Insufficient data to recommend a STEL or notations for carcinogenicity, sensitisation, or skin absorption.</p>		
DFG	NA	NA
No report.		
SCOEL	NA	NA
No report.		
OARS/AIHA	NA	NA
No report.		

Source	Year set	Standard
HCOTN	2002	TWA: 10 mg/mg³
<p>Summary of additional data:</p> <p>Current administrative TWA considered too high due to the lack of human exposure data or animal experiments regarding irritation and sensitisation, carcinogenicity, reproduction toxicity and <i>in vivo</i> genotoxicity studies. Nasal epithelial lesions considered as the critical effect, which has a reported LOAEC of 3.0 mg/m³ from a sub-chronic inhalation study. Application of a 24-fold factor to account for the absence of NOAEL, intra- and interspecies variation, and differences between experimental exposure conditions and exposure in the workplace. Following the preferred value approach, a health-based OEL of 0.1 mg/m³ is recommended.</p> <p>Human data:</p> <ul style="list-style-type: none"> • None presented <p>Animal data:</p> <ul style="list-style-type: none"> • LD₅₀: 1320 mg/kg (rats, oral) • Sub-chronic inhalation study with exposure groups 0, 2.5, 5.0, 10, 20, and 40 mg/m³ (rats, mice, 6 h/d, 5 d/wk, 2 wk): <ul style="list-style-type: none"> ○ no signs of substance-related toxicity; highest exposure concentration represents highest concentration below vapour saturation and aerosol formation ○ no histopathological changes to liver, spleen, kidney, and lungs ○ inflammatory nasal epithelium lesions noted in necropsies of all exposure groups ○ severity of lesions was dose-dependent and minimal to mild in 0.32–1.3 ppm groups • Second sub-chronic inhalation study with exposure groups 0, 3.0, 10, and 30 mg/m³ (rats, mice, 6 h/d, 5 d/wk, 13 wk): <ul style="list-style-type: none"> ○ dose-dependent nasal lesions observed in all exposure groups, as in 2 wk study ○ mean iron lung burden of highest exposure group was 4 times greater than controls (rats) ○ dose-related increase in relative liver weights (rats) in highest exposure group for and highest 2 for females; liver weight decreased in female mice • Available <i>in vivo</i> and <i>in vitro</i> mutagenicity data are equivocal. 		

Secondary source reports relied upon

NIL.

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



Source	Notations
NICNAS	NA
EU Annex	NA
ECHA	NA
ACGIH	—
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

Insufficient data to assign a skin notation.

IDLH

Is there a suitable IDLH value available? No

Additional information

Molecular weight:	186.04
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:	<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.

Health Council of the Netherlands (HCOTN) (2002) Dicyclopentadienyl iron (ferrocene). Health-based calculated occupational cancer risk values. The Hague: Health Council of the Netherlands; publication no. 2000/15OSH/047.

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