

GHS Classification

ID652

2-Cyclohexen-1-one, 3,5,5-trimethyl-

CAS 78-59-1

Date Classified: Jun. 20, 2006 (Environmental Hazards: Mar. 31, 2006)

Physical Hazards

Reference Manual: GHS Classification Manual (Feb. 10, 2006)

Hazard class	Classification	symbol	signal word	hazard statement	Rational for the classification
1 Explosives	Classification not possible	-	-	-	Classification not possible due to lack of data, though the substance contains unsaturated C-C bonds as chemical groups associated with explosive properties present.
2 Flammable gases	Not applicable	-	-	-	Liquid (GHS definition)
3 Flammable aerosols	Not applicable	-	-	-	Not aerosol products
4 Oxidizing gases	Not applicable	-	-	-	Liquid (GHS definition)
5 Gases under pressure	Not applicable	-	-	-	Liquid (GHS definition)
6 Flammable liquids	Category 4	-	Warning	Combustible liquid	Although flash point by open cup measuring device was 96.1 degC, it adopted 84 degC of flash point by a closed cup flash point analyzer device, and was classified as Category 4 (GHS standards: flash point being more than 60 degC and 93 degC or less).
7 Flammable solids	Not applicable	-	-	-	Liquid (GHS definition)
8 Self-reactive substances and mixtures	Classification not possible	-	-	-	Classification not possible due to lack of data, though the substance contains unsaturated C-C bonds as chemical groups with self-reactive properties present.
9 Pyrophoric liquids	Not classified	-	-	-	The ignition points is 460 - 462 degC (ICSC (J) (2000), pocket book books (1997))
10 Pyrophoric solids	Not applicable	-	-	-	Liquid (GHS definition)
11 Self-heating substances and mixtures	Classification not possible	-	-	-	Test methods applicable to liquid substances are not available
12 Substances and mixtures, which in contact with water, emit flammable gases	Not applicable	-	-	-	The chemical structure of the substance does not contain metals or metalloids(B, Si, P, Ge, As, Se, Sn, Sb, Te, Bi, Po, At).
13 Oxidizing liquids	Not applicable	-	-	-	Organic compounds containing oxygen (but not chlorine and fluorine) chemically bonded only to carbon (but not to other elements).
14 Oxidizing solids	Not applicable	-	-	-	Liquid (GHS definition)
15 Organic peroxides	Not applicable	-	-	-	Organic compounds containing no -O-O- structure
16 Corrosive to metals	Classification not possible	-	-	-	No data available

Health Hazards

Hazard class	Classification	symbol	signal word	hazard statement	Rational for the classification
1 Acute toxicity (oral)	Category 4	Exclamation mark	Warning	Harmful if swallowed	It was set as Category 4 based on rat LD50 = 1843mg/kg: calculated by the technical guideline using seven data of rat (SIDS (2003), EHC 174 (1995)).
1 Acute toxicity (dermal)	Category 4	Exclamation mark	Warning	Harmful in contact with skin	LD50 = 1265mg/kg calculated by the technical guideline using 4 examination of rabbits (SIDS (2003), PATTY (5th, 2001)). And LD50 = 1700mg/kg (SIDS (2003)) of a rat examination. It was set as Category 4 based on the lower value.
1 Acute toxicity (inhalation: gas)	Not applicable	-	-	-	Liquid (GHS definition)
1 Acute toxicity (inhalation: vapour)	Classification not possible	-	-	-	Classification not possible due to lack of data
1 Acute toxicity (inhalation: dust, mist)	Category 5	-	Warning	May be harmful if inhaled	It done by higher concentrations than the saturated vapor pressure pressures concentrations, and based on LC50 = 7mg/L (SIDS (2003)) of the rat inhalation test considered to be mist tests. So it was set as Category 5
2 Skin corrosion / irritation	Category 3	-	Warning	Causes mild skin irritation	Based on the report that in test of less than 4 hours on rabbits or guinea pigs, there was mild skin irritation or no stimulativeness observed (SIDS (2003), EHC 174 (1995), PATTY (5th, 2001)), it was classified as Category 3.
3 Serious eye damage / eye irritation	Category 2A-2B	Exclamation mark	Warning	Causes serious eye irritation	There is the statement that humans had eye irritation (ACGIH (2001), SIDS (2003)), and that there was moderate or mild eye irritation (SIDS(2003), EHC 174 (1995)), and that although moderate to severe impairment was produced, it recovered within 14 days in rabbit test (SIDS (2003)). So it was set as Category 2A-2B.
4 Respiratory/skin sensitization	respiratory sensitization: Classification not possible; Skin sensitization: Not classified	(Respiratory sensitization)-; (Skin sensitization)-	(Respiratory sensitization)-; (Skin sensitization)-	(Respiratory sensitization)-; (Skin sensitization)-	Respiratory sensitization: No data. Skin sensitization: Based on the statements that sensitization was not identified in guinea pigs tests [SIDS (2003) and EHC 174 (1995)] and that there is no sensitization in humans(SIDS (2003), ECETOC JACC 10 (1989)), it was put outside of the Category.
5 Germ cell mutagenicity	Not classified	-	-	-	The lack of results for human over generation epidemiology, the over generation mutagenicity test, and the productive cell in vivo mutagenicity test, and based on the statement that it gave negative by two in vivo somatic mutagenicity examinations (mouse bone marrow cells micronucleus test) (SIDS (2003), EHC 174 (1995), ECETOC JACC 10 (1989)). So we classified it as Out Of Category by the technical guideline.

6	Carcinogenicity	Category 2	Health hazard	Warning	Suspected of causing cancer (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)	It was set as 2. Based on being classified into A3 according to ACGIH (ACGIH (2001)), and being classified into a category 3 by EU and R40 being given (EU-Annex I (2005)).
7	Toxic to reproduction	Not classified	-	-	-	Since it is not observed that adverse effects on genital tract and fetal development in the rat or mouse test (SIDS (2003), EHC 174 (1995), PATTY (5th, 2001)) and the dog study (SIDS (2003)), it is considered as on the outside of
8	Specific target organs/systemic toxicity following single exposure	Category 3 (respiratory tract irritation, narcotic effects)	Exclamation mark	Warning	may cause respiratory irritation or may cause drowsiness and dizziness (respiratory tract irritation, narcotic effects)	There is the respiratory irritation (irritation of nose and throat) and anesthetic action (nausea, headache, dizziness, faint, choking sensation) (ACGIH (2001), EHC 174 (1995)) in human exposure report. And there is the description that there is respiratory irritation also in rat and rabbit (EHC 174 (1995)) and there are symptoms which indicate anesthetic action such as ataxia, suppression state and coma (EHC 174 (1995), SIDS (2003)). So it is classified into Category 3 (respiratory irritation and anesthetic action)
9	Specific target organs/systemic toxicity following repeated exposure	Classification not possible	-	-	-	In the example of exposure in the humans mentioned of SIDS (2003), effects to specific organ is not admitted, but only fatigue and malaise are reported. In an animal examination, serious effects on specific organ is not admitted by oral dosage higher than the guidance value of Category 2 (SIDS (2003), EHC 174 (1995)). However, the affect (bleeding, edema, inflammatory, changes in the tissue) on lungs and the affect (changes in the tissues) on the kidney are mentioned with higher dosage than the guidance value of 2 in the inhalation test of the animal (EHC 174 (1995), PATTY (5th, 2001)). In order that there might be no data which serves as a conclusive factor of a classification among the above informations, it was presupposed that it cannot be classified.
10	Aspiration hazard	Classification not possible	-	-	-	No data available

Environmental Hazards

Hazard class	Classification	symbol	signal word	hazard statement	Rational for the classification
11 Hazardous to the aquatic environment (acute)	Category 3	-	-	Harmful to aquatic life	It was classified into Category 3 from 96-hour LC50=12.9mg/L of Crustacea (Mysid shrimp) (SIDS, 2005).
11 Hazardous to the aquatic environment (chronic)	Not classified	-	-	-	Since rapidly degrading (28-day decomposition rate of the OECD test guideline 301A: 95% (SIDS, 2003)), and less bio-accumulative (BCF=1.8 (Existing Chemicals Safety Check Data)).