GHS Classification

ID986 butenone

CAS 78-94-4 Date Classified: Aug. 18, 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	Not applicable	–	–	–	There are no chemical groups associated with explosive properties present in the molecules.
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 1	Flame	Danger	Extremely flammable liquid and vapour	UNRTDG Subsidiary risks Class: 3, 8, PG I
7	Flammable solids	Not applicable	–	–	–	Liquid (GHS definition)
8	Self-reactive substances and mixtures	Type G	–	–	–	UNRTDG Non-hazardrous Substance
9	Pyrophoric liquids	Not classified	–	–	–	Not ignite spontaneously on coming into contact with air at normal temperatures
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 metaloids(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 and hydrogen (but not to other elements).
14	Oxidizing solids	Not applicable	–	–	–	Liquid (GHS definition)
15	Organic peroxides	Not applicable	–	–	–	Containing no -O-O- structure
16	Corrosive to metals	Classification not possible	–	–	–	Classification not possible due to lack of data

Health Hazards

	Hazard class	Classification	symbol	signal word	hazard statement	Rational for the classification
1	Acute toxicity (oral)	Category 2	Skull and crossbones	Danger	Fatal if swallowed	Rat LD50 value: 23.1mg/kg (ACGIH 7th, 2001), 31mg/kg, about 30mg/kg, about 22mg/kg (DFGOT vol.9, 1998). Calculated based on the data above. Since the calculated values was 22.7mg/kg, it was classified to category 2.
1	Acute toxicity (dermal)	Category 1	Skull and crossbones	Danger	Fatal in contact with skin	It was set as Category 1. Based on the description that three among three cases died by dermal administration of 0.2mg/kg and 0.05mg/kg to rabbits (DFGOT (vol.9, 1998)).
1	Acute toxicity (inhalation: gas)	Not applicable	–	–	–	Liquid (GHS definition)
1	Acute toxicity (inhalation: vapour)	Category 1	Skull and crossbones	Danger	Fatal if inhaled	Lower value was adopted from rat LC50 (4 hours): 0.007mg/L (2.4ppm) (ACGIH 7th, 2001) and 22.4ppm (equivalent 0.0641mg/L) (DFGOT vol.9, 1998). 2.4 ppm was considered as the steam with almost no mist from vapor pressure. And classified as Category 1 by the ppm concentration standard.
1	Acute toxicity (inhalation: dust, mist)	Classification not possible	–	–	–	No data available
2	Skin corrosion / irritation	Category 1A-1C	Corrosion	Danger	Causes severe skin burns and eye damage	In the test applied to the skin of the rabbit, from description that inflammatory changes were seen and the serious necrosis (severe necrosis) appeared 1.5 and 15 minutes after apply (DFGOT (9 vol. 1998)), it was judged that there was caustic and was set as Category 1A-1C. [display] It is more desirable to be set as 1A from a viewpoint of safety, when subdivision is necessary to be carried out.
3	Serious eye damage / eye irritation	Category 1	Corrosion	Danger	Causes serious eye damage	It had corrosiveness to the skin. And there is the description that very severe corneal degeneration was acknowledged in the test applied to the eyes of the rabbits (DFGOT (vol.9, 1998)). So we classified it as Category 1.
4	Respiratory/skin sensitization	Respiratory sensitization: Classification not possible; Skin sensitization: Category1	(Respiratory sensitization)-; (Skin sensitization)Exclamation mark	(Respiratory sensitization)-; (Skin sensitization)Warning	(Respiratory sensitization)-; (Skin sensitization)May cause allergic skin reaction	Respiratory sensitization: No data. Skin sensitization : We found a description that there was a report of one case in which sensitizing was acknowledged in DFGOT (vol.9, 1998). Moreover, since it is classified into SEN (ACGIH 7th, 2001) according to ACGIH and was classified into Sh (MAK/BAT, 2004) according to DFG, we classified it to be Category 1. Furthermore, DFGOT (vol.9, 1998) has description that severe contact dermatitis was acknowledged in Open Epicutaneous Test which used the guinea pigs.
5	Germ cell mutagenicity	Classification not possible	–	–	–	There is the result that the small core examination which used the male rat bone marrow cell of NTP DB (2006) is equivocal, and the result of the micronucleus test which used mouse peripheral blood is negative for a female and equivocal for a male. So it cannot classify according to the shortage of data.
6	Carcinogenicity	Classification not possible	–	–	–	No data available

7	Toxic to reproduction	Classification not possible	–	–	–	No data available
8	Specific target organs/systemic toxicity following single exposure	Category 1 (respiratory organs, kidneys); Category 3 (narcotic effects)	Health hazard; Exclamation mark	Danger	Cause damage to organs (respiratory organs, kidneys); May cause respiratory irritation or may cause drowsiness and dizziness (narcotic effects)	Because of a description in DFGOT (vol.9, 1998) referring to that effects on respiratory systems were confirmed at concentration within the limits of guidance value of Category 1 through an inhalation exposure test using rats, rabbits, cats, guinea pigs, and mice, and of a description in DFGOT (vol.9, 1998) referring to confirmation of renal damage at a dosage within the limits of guidance value of Category 1 in oral administration studies with rabbits and cats. So it was judged as Category 1 (respiratory organs, kidney). Moreover, it was judged as Category 3 (anesthetic actions) because of a description in DFGOT (vol.9, 1998) referring to that flexion reflex inhibition was confirmed in a inhalation exposure test using rabbits, and of a description in ACGIH (7th, 2001) indicating anesthetic actions as effects on humans.
9	Specific target organs/systemic toxicity following repeated exposure	Category 1 (respiratory organs)	Health hazard	Danger	Causes damage to organs (respiratory organs) through prolonged or repeated exposure	It was classified into Category 1 (respiratory tracts) based on description that dyspnea was observed with concentration within the guidance value range for Category 1 in the inhalation exposure test on rats (DFGOT (vol.9, 1998)).
10	Aspiration hazard	Category 2	Health hazard	Warning	May be harmful if swallowed and enters airways	Category 2 because of a ketone composed of 13 carbon atoms or less.

Environmental Hazards

Hazard class	Classification	symbol	signal word	hazard statement	Rational for the classification
11 Hazardous to the aquatic environment (acute)	Category 1	Environment	Warning	Very toxic to aquatic life	It was classified into Category 1 from 96-hour EC50=120microg/L of algae (Selenastrum) (AQUIRE, 2003).
11 Hazardous to the aquatic environment (chronic)	Category 1	Environment	Warning	Very toxic to aquatic life with long lasting effects	Classified into Category 1, since acute toxicity was Category 1, not rapidly degrading (BOD :1%(BUA233, 2001)), though supposed less bioaccumulative(log Kow=0.41(PHYSPROP Database, 2005)).