

GHS Classification

ID747

Diacetone alcohol

CAS 123-42-2

Date Classified: Jul. 24, 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 4	-	Warning	Combustible liquid	Since flash point of reagent grades was 66 degC, it was classified as Category 4. (Since industrial pure product diacetone alcohol includes acetone, there is also data that indicates 8 degC of flash point. Therefore, it is class 3 Division II and III in the UN Recommendations. Such commercial items with low flash point are classified as Category 2).
7 Flammable solids	Not applicable	-	-	-	Liquid (GHS definition)
8 Self-reactive substances and mixtures	Not applicable	-	-	-	There are no chemical groups associated with explosive or self-reactive properties present in the molecule.
9 Pyrophoric liquids	Not applicable	-	-	-	The ignition points is 603 degC and there is no spontaneous combustibility in 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 metalloids(B, Si, P, Ge, As, Se, Sn, Sb, Te, Bi, Po, At).
13 Oxidizing liquids	Not applicable	-	-	-	Organic compounds containing oxygen 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	-	-	-	Organic compounds containing no -O-O- structure
16 Corrosive to metals	Classification not possible	-	-	-	No data available on corrosion to metals

Health Hazards

Hazard class	Classification	symbol	signal word	hazard statement	Rational for the classification
1 Acute toxicity (oral)	Category 5	-	Warning	May be harmful if swallowed	SPECIES: Rat ENDPOINT: LD50 VALUE: 4000 mg/kg REFERENCE SOURCE: SIDS (2000)
1 Acute toxicity (dermal)	Not classified	-	-	-	Since the value (SIDS (2000)) of rabbit LD50= 13630mg/kg had exceeded 5000mg/kg (Category 5), it was set as the outside of Category.
1 Acute toxicity (inhalation: gas)	Not applicable	-	-	-	Liquid (GHS definition)
1 Acute toxicity (inhalation: vapour)	Classification not possible	-	-	-	Since there is no LC50 value, it cannot be classified. (It is assumed to be Category 3 to out of Category, since no death was observed on rats with 7.23g/m3 (1520ppm) (SIDS (2000)))
1 Acute toxicity (inhalation: dust, mist)	Classification not possible	-	-	-	No data available
2 Skin corrosion / irritation	Category 2	Exclamation mark	Warning	Causes skin irritation	It was classified as Category 2 based on the information of moderate irritation in irritation test on rabbits (SIDS (2000)).
3 Serious eye damage / eye irritation	Category 2A	Exclamation mark	Warning	Causes serious eye irritation	It was set as Category 2A using information of moderate or highly irritating with a rabbit (SIDS (2000), PATTY (5th, 2001)), and that there is irritation with humans (SIDS (2000), ACGIH (2001)).
4 Respiratory/skin sensitization	respiratory sensitization: Classification not possible; Skin sensitization: Classification not possible	(Respiratory sensitization)-; (Skin sensitization)-	(Respiratory sensitization)-; (Skin sensitization)-	(Respiratory sensitization)-; (Skin sensitization)-	No data available
5 Germ cell mutagenicity	Classification not possible	-	-	-	There were reports that it gave negative in vitro (SIDS (2000), PATTY (5th, 2001)), however, there was no in vivo information. Therefore we could not classify it.
6 Carcinogenicity	Classification not possible	-	-	-	Since there is no information and other test data by evaluation organizations, it cannot be classified.
7 Toxic to reproduction	Category 2	Health hazard	Warning	Suspected of damaging fertility or the unborn child	Since it is observed of declines conception rate, implantation count and implantation rate of reproductive potential and declines of total newborn count, delivery rate, neonatal count, live birth index, 4-days neonatal survival count and viability index on day 4 of offspring development (SIDS 2000)), it is classified into category 2.

8	Specific target organs/systemic toxicity following single exposure	Category 1 (respiratory); Category 2 (liver); Category 3 (narcotic effects)	Health hazard; Exclamation mark	Danger; Warning	Cause damage to organs (respiratory); May cause damage to organs (liver); May cause respiratory irritation or may cause drowsiness and dizziness (narcotic effects)	Since respiratory irritations and pulmonary diseases (SIDS (2000), ACGIH (2001)) are seen in human cases, it was set as Category 1 (respiratory system), and by the data that cases of liver is seen by 2ml/kg (equivalent : 1860mg/kg) rat oral taking (ACGIH (2001), PATTY (5th, 2001)), so it was set as category 2 (liver) from a guidance value. Since the anesthetic actions was seen in the animal (ACGIH (2001), PATTY (5th, 2001)), it is classified into Category 3.
9	Specific target organs/systemic toxicity following repeated exposure	Category 1 (kidneys)	Health hazard	Danger	Causes damage to organs (kidneys) through prolonged or repeated	It was classified into Category 1 (kidney) according to the description that "onset of nephrotic syndrome is used as the evidence of proliferative glomerulonephritis." in example of accident of humans at diacetone alcohol and ethanol exposure (PATTY (5th, 2001)).
10	Aspiration hazard	Classification not possible	-	-	-	No data available on chemical pneumonia

Environmental Hazards

Hazard class	Classification	symbol	signal word	hazard statement	Rational for the classification
11 Hazardous to the aquatic environment (acute)	Not classified	-	-	-	it carried out the outside of Category from 96-hour LC50>100mg/L of fishes (<i>Oryzias latipes</i>), and others (MOE eco-toxicity tests of chemicals, 1996).
11 Hazardous to the aquatic environment (chronic)	Not classified	-	-	-	Since not water-insoluble (water solubility=1.00*106mg/L(PHYSROP Database, 2005)) and acute toxicity is low.