GHS Classification

ID550 tert-Butyl hydroperoxide

CAS 75-91-2 Date Classified: Sep. 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 on the kick-off temperature and decomposition energy, though being a peroxide with its oxygen budget calculated at −195. Heating may cause an explosion according to HSDB (2006).
2	Flammable gases	Not applicable	—	—	—	Classified as "liquid" according to GHS definition
3	Flammable aerosols	Not applicable	—	—	—	Not aerosol products
4	Oxidizing gases	Not applicable	—	—	—	Classified as "liquid" according to GHS definition
5	Gases under pressure	Not applicable	—	—	—	Classified as "liquid" according to GHS definition
6	Flammable liquids	Category 2	Flame	Danger	Highly flammable liquid and vapour	Because of a lack of data on the flash point. The substance can be classified into Category 2 or 3 with the flash point of <27degC (c.c.) (NFPA (13th, 2002)) and the boiling point of 89degC (decomposition) (Lide (84th, 2003)), and is placed in "Category 2" from the viewpoint of safety.
7	Flammable solids	Not applicable	—	—	—	Classified as "liquid" according to GHS definition
8	Self-reactive substances and mixtures	Not applicable	—	—	—	Classified as "organic peroxides" though being a peroxide containing chemical groups with explosive properties. Classified into Division 5.2 by the UN Recommendation on the Transport of Dangerous Goods (UN numbers (3103, 3105, 3107, 3109) are given only to those diluted according to their concentrations and proportions of diluents; tert-butyl hydroperoxide in neat liquid is prohibited for transport and thus has no UN number).
9	Pyrophoric liquids	Classification not possible	—	—	—	Classification not possible due to lack of data, though heating may cause a fire according to HSDB (2006).
10	Pyrophoric solids	Not applicable	—	—	—	Classified as "liquid" according to 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	—	—	—	Containing no metals or metalloids (B, Si, P, Ge, As, Se, Sn, Sb, Te, Bi, Po, At)
13	Oxidizing liquids	Classification not possible	—	—	—	Classification not possible due to lack of data, though being organic compounds containing oxygen bound to the elements other than carbon and hydrogen, and classified as a powerful oxidant according to HSDB (2006).
14	Oxidizing solids	Not applicable	—	—	—	Classified as "liquid" according to GHS definition
15	Organic peroxides	Type A	Bomb explosion	Danger	Heating may cause an explosion	Type classification is not possible due to lack of data, though organic compounds containing "O-O" structure, with active oxygen quantity calculated at 35.5%, that is, "Organic peroxides." Organic peroxides permitted for transport are assigned general entries by the UN Recommendation on the Transport of Dangerous Goods. As for tert-butyl hydroperoxide, only those diluted are given UN numbers (3103, 3105, 3107, 3109), subclassified into "Type C," "Type D," "Type E" and "Type F" according to their concentrations and proportions of diluents. Since those undiluted are interpreted as "Type A" (prohibited for transport), tert-butyl hydroperoxide (in neat liquid) is classified as "Type A" by GHS classification. Those diluted are assigned to Division 5.2 (UN#3103 Organic peroxides Type C (liquid), UN#3105 Organic peroxides Type D (liquid), UN#3107 Organic peroxides Type E (liquid) and UN#3109 Organic peroxides Type F (liquid)) by the UN Recommendation on the Transport of Dangerous Goods.
16	Corrosive to metals	Classification not possible	—	—	—	No data available. Under the UN Recommendation on the Transport of Dangerous Goods, those diluted substances classified as "Organic peroxides" need to be labeled with the subsidiary risk label of "Corrosive Substances." However, the category includes skin corrosivity, and it is unclear whether the substance is classified as "metal" corrosive (UN numbers of those in solution: UN#3103 Organic peroxides Type C (liquid), UN#3105 Organic peroxides Type D (liquid), UN#3107 Organic peroxides Type E (liquid) and UN#3109 Organic peroxides Type F (liquid)).

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	Based on the rat LD50 (oral route) value of 560mg/kg (SIDS (1995)).
1	Acute toxicity (dermal)	Category 3	Skull and crossbones	Danger	Toxic in contact with skin	Based on the LD50 value of 470mg/kg representing the lower of the two testing data, rabbit LD50 (dermal route) of 628mg/kg (SIDS (1995)) and rat LD50 (dermal route) of 470mg/kg (PATTY (4th, 1999)).
1	Acute toxicity (inhalation: gas)	Not applicable	—	—	—	Due to the fact that the substance is "liquid" according to the GHS definition and inhalation of its gas is not expected.
1	Acute toxicity (inhalation: vapour)	Category 3	Skull and crossbones	Danger	Toxic if inhaled	Based on the rat LC50 (inhalation of vapour) value of 502ppm (PATTY (4th, 1999)) was lower than 90% of the saturated vapour concentration (27,000ppm) under a saturated vapour pressure of 2.7kPa (20degC), the substance was considered as "vapour containing substantially no mist" and was classified based on standard values expressed in ppm.
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	Based on the description in the report on rat skin irritation tests (PATTY (4th, 1999)): "Causes very strong irritation." Although classified into Category 1A-1C, the substance should be placed in Category 1A from the viewpoint of safety if further subclassification is needed.
3	Serious eye damage / eye irritation	Category 1	Corrosion	Danger	Causes serious eye damage	Based on the description in the report on rat eye irritation tests (PATTY (4th, 1999)): "Causes very strong irritation." Also based on the description in ICSC (1999) of human health effects: "redness, pains and deep burn." The substance is thus considered corrosive to the eye.
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)—	Respiratory sensitization: No data available Skin sensitization: No data available

5	Germ cell mutagenicity	Category 2	Health hazard	Warning	Suspected of causing genetic defects	Based on negative and positive data on multi-generation mutagenicity tests (dominant lethal tests) and somatic cell mutagenicity tests in vivo (chromosome aberration tests), and the absence of data on germ cell mutagenicity tests in vivo, described in SIDS (1995), DFGOT Vol. 3 (1992) and NTP DB (Access on June, 2006). The results of dominant lethal tests were not based on the sound knowledge, whereas the positive data on chromosome aberration tests in vivo were considered not to be definitive. However, all the in vitro tests (Ames assay, chromosome aberration assay, mouse lymphoma) were positive for mutagenicity, and therefore the substance is classified into Category 2.
6	Carcinogenicity	Classification not possible	—	—	—	Insufficient data available
7	Toxic to reproduction	Not classified	—	—	—	Based on no evidence of adverse effects on parental reproduction and pup development in combined studies and teratogenicity studies, described in SIDS (1995).
8	Specific target organs/systemic toxicity following single exposure	Category 2 (nervous system, blood system, respiratory organs) Category 3 (narcotic effects)	Health hazard	Warning	May cause damage to organs (nervous system, blood system, respiratory organs) (Narcotic effects) May cause drowsiness or dizziness	Based on the evidence from animal studies: "clinical signs including hypoactivity and lacrimation...loss of righting reflex...signs of hematuria" (PATTY (4th, 1999)) , "hypoactivity...loss of righting reflex, lacrimation...hematuria" (IUCLID (1999)), "methemoglobinemia or carboxyhemoglobin," "cyanosis" (RTECS (2006)), "decreased respiratory rate and apnea" (IUCLID (1999)). The effects on experimental animals were observed at dosing levels within the guidance value ranges for Category 2 (nervous system, blood system) and Category 1 (respiratory organs). However, the referenced study for the respiratory effects has a priority rating of 2, which does not meet the criteria for 1b (3) specified in the "Technical Guideline for GHS Health Hazard Classification," therefore these are classified into Category 2.
9	Specific target organs/systemic toxicity following repeated exposure	Category 1 (kidneys) Category 2 (blood system)	Health hazard	Danger	Causes damage to organs through prolonged or repeated exposure (kidneys) May cause damage to organs through prolonged or repeated exposure (blood system)	Based on the evidence from animal studies including "reticulocytopenia, increased bilirubin level, and nephrosis" (SIDS (1995)). The effects on experimental animals were observed at dosing levels within the guidance value ranges for Category 1 (kidneys) and Category 2 (blood system).
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 2	-	-	Toxic to aquatic life	It was classified into Category 2 from 3 day ErC50=2.1mg/L of the algae (Selenastrum) (IUCLID, 2000).
11	Hazardous to the aquatic environment (chronic)	Category 2	Environment	-	Toxic to aquatic life with long lasting effects	Although acute toxicity was Category 2 and the bio-accumulation potential was low (BCF=1.8(Existing Chemical Safety Inspections Data)), since there was no rapidly degrading (the decomposition by BOD: 0%(Existing Chemical Safety Inspections Data)), it was classified into Category 2.