SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : tert-Butyl acetate
Catalog Number : io-1877
CAS Number : 540-88-5
Identified uses : Laboratory chemicals, manufacture of chemical compounds
Company : Ionz

>> R&D Use only

2. Hazards Identification

GHS Classification:

Flammable liquid (category 2)
Acute toxicity, oral (Category 3)
Acute toxicity, dermal (Category 3)
Acute toxicity, inhalation (Category 3)
Specific target organ toxicity, single exposure (Category 1)

Note

>> Pictograms displayed are for > 99.9% (1391 of 1392) of reports that indicate hazard statements. This chemical does not meet GHS hazard criteria for < 0.1% (1 of 1392) of reports.

Pictogram(s)

GHS Hazard Statements

>> H225 (> 99.9%): Highly Flammable liquid and vapor [Danger Flammable liquids]

>> H332 (34.5%): Harmful if inhaled [Warning Acute toxicity, inhalation]

Precautionary Statement Codes

>> P210, P233, P240, P241, P242, P243, P261, P271, P280, P303+P361+P353, P304+P340, P317, P370+P378, P403+P235, and P501

NFPA 704 Diamond

NFPA Health Rating

>> 1 - Materials that, under emergency conditions, can cause significant irritation.

NFPA Fire Rating

>> 3 - Liquids and solids that can be ignited under almost all ambient temperature conditions. Materials produce hazardous atmospheres with air under almost all ambient temperatures or, though unaffected by ambient temperatures, are readily ignited under almost all conditions.

NFPA Instability Rating

>> 0 - Materials that in themselves are normally stable, even under fire conditions.

Health Hazards:

>> INHALATION: Irritation of throat. EYES: Irritation. (USCG, 1999)

>> Excerpt from ERG Guide 129 [Flammable Liquids (Water-Miscible / Noxious)]:

>> HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along the ground and collect in low or confined areas (sewers, basements, tanks, etc.). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids will float on water. (ERG, 2024)

>> Highly flammable. Above 15.5 °C explosive vapour/air mixtures may be formed.

3. Composition/Information On Ingredients

Chemical name : tert-Butyl acetate
CAS Number : 540-88-5
Molecular Formula : C6H12O2
Molecular Weight : 116.1600 g/mol

4. First Aid Measures

First Aid:

>> Excerpt from NIOSH Pocket Guide for tert-Butyl acetate:

>> Eye: IRRIGATE IMMEDIATELY - If this chemical contacts the eyes, immediately wash (irrigate) the eyes with large amounts of water, occasionally lifting the lower and upper lids. Get medical attention immediately.

>> Skin: WATER FLUSH PROMPTLY - If this chemical contacts the skin, flush the contaminated skin with water promptly. If this chemical penetrates the clothing, immediately remove the clothing and flush the skin with water promptly. If irritation persists after washing, get medical attention.

>> Breathing: RESPIRATORY SUPPORT - If a person breathes large amounts of this chemical, move the exposed person to fresh air at once. If breathing has stopped, perform artificial respiration. Keep the affected person warm and at rest. Get medical attention as soon as possible.

>> Swallow: MEDICAL ATTENTION IMMEDIATELY - If this chemical has been swallowed, get medical attention immediately. (NIOSH, 2024)

First Aid Measures

Inhalation First Aid

>> Fresh air, rest.

Skin First Aid

>> Remove contaminated clothes. Rinse and then wash skin with water and soap.

Eye First Aid

>> First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Ingestion First Aid

>> Rinse mouth.

5. Fire Fighting Measures

>> Fire Extinguishing Agents Not to Be Used: Water may be ineffective.

>> Fire Extinguishing Agents: Alcohol foam, CO2, dry chemical (USCG, 1999)

>> Use carbon dioxide, dry powder, foam. In case of fire: keep drums, etc., cool by spraying with water.

6. Accidental Release Measures

Isolation and Evacuation:

Isolation and evacuation measures to take when a large amount of this chemical is accidentally released in an emergency.

>> Excerpt from ERG Guide 129 [Flammable Liquids (Water-Miscible / Noxious)]:

>> IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area for at least 50 meters (150 feet) in all directions.

>> LARGE SPILL: Consider initial downwind evacuation for at least 300 meters (1000 feet).

>> FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

Spillage Disposal:

Methods for containment and safety measures to protect workers dealing with a spillage of this chemical.

>> Do NOT wash away into sewer. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

7. Handling And Storage

Safe Storage:

>> Fireproof. Separated from strong oxidants, strong bases and strong acids.

8. Exposure Control/ Personal Protection

REL-TWA (Time Weighted Average)

>> 200 ppm (950 mg/m³)

>> TWA 200 ppm (950 mg/m3)

>> 200.0 [ppm]

PEL-TWA (8-Hour Time Weighted Average)

>> 200 ppm (950 mg/m³)

>> 50.0 [ppm]

TLV-STEL

>> 150.0 [ppm]

>> 50 ppm as TWA; 150 ppm as STEL.

TLV-TWA (Time Weighted Average)

>> 50 ppm [2009]

TLV-STEL (Short Term Exposure Limit)

>> 150 ppm [2009]

MAK (Maximale Arbeitsplatz Konzentration)

>> 96 mg/m

Inhalation Risk:

>> A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20 °C.

Effects of Short Term Exposure:

>> The vapour is irritating to the respiratory tract. The substance is mildly irritating to the eyes and skin. Exposure far above the OEL could cause lowering of consciousness.

Effects of Long Term Exposure:

>> The substance defats the skin, which may cause dryness or cracking.

Fire Prevention

>> NO open flames, NO sparks and NO smoking. Above 15.5 °C use a closed system, ventilation and explosion-proof electrical equipment.

Inhalation Prevention

>> Use ventilation, local exhaust or breathing protection.

Skin Prevention

>> Protective gloves.

Eye Prevention

>> Wear safety spectacles or eye protection in combination with breathing protection.

Ingestion Prevention

>> Do not eat, drink, or smoke during work.

Exposure Control and Personal Protection

Maximum Allowable Concentration (MAK)

>> 20.0 [ppm]

9. Physical And Chemical Properties

Molecular Weight:

>> 116.16

Exact Mass:

>> 116.083729621

Physical Description:

>> Tert-butyl acetate is a colorless liquid with a mild odor. Floats on water. Produces irritating vapor. (USCG, 1999)

>> COLOURLESS LIQUID WITH CHARACTERISTIC ODOUR.

Color/Form:

>> Liquid

Odor:

>> Fruity odor

Boiling Point:

>> 208 °F at 760 mmHg (USCG, 1999)

>> 97.8 °C

Flash Point:

>> 72 °F (NIOSH, 2024)

>> 15.5 °C c.c.

Solubility:

>> Insoluble (NIOSH, 2024)

>> Solubility in water: poor

Density:

>> 0.8665 at 68 °F 0.8593 at 25 °C (USCG, 1999) - Less dense than water; will float

>> Relative density (water = 1): 0.86

Vapor Density:

>> 4.0 at BP (Air = 1)

>> Relative vapor density (air = 1): 4

Vapor Pressure:

>> 47.0 [mmHg]

>> Vapor pressure, kPa at 25 °C: 6.3

LogP:

>> log Kow = 1.76

>> 1.76

Stability/Shelf Life:

>> Heat /contributes to instability/.

Autoignition Temperature:

>> 799 °F (425 °C) /Butyl acetate/

Decomposition:

>> When heated to decomposition it emits acrid smoke and irritating fumes.

Heat of Vaporization:

>> 33.07 kJ/mol at bp; 39.03 kJ/mol at 25 °C

Odor Threshold:

>> Odor Threshold Low: 4.0 [mmHg]

>> Odor Threshold High: 47.0 [mmHg]

>> Odor threshold from "Quick Guide: The Electronic NIOSH Pocket Guide to Chemical Hazards"

Refractive Index:

>> Index of refraction: 1.3855 at 20 °C

10. Stability And Reactivity

>> Highly flammable. Insoluble in water.

>> Highly Flammable

11. Toxicological Information

Exposure Routes:

>> The substance can be absorbed into the body by inhalation of its vapour.

>> inhalation, ingestion, skin and/or eye contact

Inhalation Exposure

>> Cough. Sore throat.

Skin Exposure

>> Dry skin.

Eye Exposure

>> Redness. Pain.

>> Itch, inflammation eyes; irritation upper resp tract; headache; narcosis; dermatitis

Target Organs:

Organs that are affected by exposure to this chemical. Information in this section reflects human data unless otherwise noted.

>> respiratory system, eyes, skin, central nervous system

Adverse Effects:

An adverse effect is an undesired harmful effect resulting from a medical treatment or other intervention.

>> Neurotoxin - Acute solvent syndrome

>> Occupational hepatotoxin - Secondary hepatotoxins: the potential for toxic effect in the occupational setting is based on cases of poisoning by human ingestion or animal experimentation.

Antidote and Emergency Treatment:

>> Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Esters and related compounds/

Human Toxicity Excerpts:

>> /HUMAN EXPOSURE STUDIES/ A study of sensory irritation (nasal pungency) associated with a series of homologous ketones and secondary and tertiary alcohols and esters was conducted. The study group consisted of three men and one woman, 41 to 65 years old, who lacked a sense of smell (anosmics) and three men and one woman 41 to 68 years old, with normal olfaction (normosmics). The subjects were exposed to 2-propanone (67641), 2-pentanone (107879), 2-heptanone (110430), 2-nonanone (821556), 2-propanol (67630), 2-methyl-2-propanol (75650), 2-butanol (78922), 4-heptanol (589559), tert-butyl-acetate (540885), and sec-butyl-acetate (105464) vapors at concentrations of 1x10-2 to 1x10+6 ppm by sniffing bottles containing the solvents. They also sniffed bottles containing a blank (nonodoriferous solvent). The subjects were asked to estimate the concentration of each solvent at which they could first detect the odor and perceive nasal pungency. Attempts were made to correlate the thresholds with the concentration of the saturated vapor at ambient temperature (23 °C). Both the normosmics and anosmics could detect the solvent vapors; however, the normosmics detected the vapors at much lower concentrations. The nasal pungency and odor thresholds of the ketones decreased with increasing carbon chain length, but tended to plateau at 2-heptanone. The odor and pungency thresholds of the alcohols tended to increase when the hydroxy group was changed from a primary to a secondary carbon atom. The odor and pungency thresholds of the esters were similar. When plotted against the logarithm of the saturation vapor concentration, the logarithm of the pungency thresholds of the compounds conformed to a linear function that was approximately parallel to the saturation vapor concentration. No association between odor threshold and saturation vapor concentration was seen. The authors conclude that anosmics as well as normosmics can detect odors of volatile organic compounds, although at different concentrations. The pungency threshold data suggest that physical rather than chemical factors are involved in the interaction of volatile organic compounds with the nasal mucosa.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ Exposure to a concentration of 10000 ppm for 5 hr caused irritation and death in guinea-pigs.

12. Ecological Information

Resident Soil (mg/kg)

>> 8.10e+00

Industrial Soil (mg/kg)

>> 3.60e+01

Resident Air (ug/m3)

>> 2.20e+00

Industrial Air (ug/m3)

>> 9.40e+00

Tapwater (ug/L)

>> 3.30e+00

MCL (ug/L)

>> 1.00e+02

Risk-based SSL (mg/kg)

>> 7.60e-04

Oral Slope Factor (mg/kg-day)-1

>> 5.00e-03

Inhalation Unit Risk (ug/m3)-1

>> 1.3e-06

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

13. Disposal Considerations

Spillage Disposal

>> Do NOT wash away into sewer. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Disposal Methods

>> SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal and plant life; and conformance with environmental and public health regulations.

>> SRP: Wastewater from contaminant suppression, cleaning of protective clothing/equipment, or contaminated sites should be contained and evaluated for subject chemical or decomposition product concentrations. Concentrations shall be lower than applicable environmental discharge or disposal criteria. Alternatively, pretreatment and/or discharge to a permitted wastewater treatment facility is acceptable only after review by the governing authority and assurance that "pass through" violations will not occur. Due consideration shall be given to remediation worker exposure (inhalation, dermal and ingestion) as well as fate during treatment, transfer and disposal. If it is not practicable to manage the chemical in this fashion, it must be evaluated in accordance with EPA 40 CFR Part 261, specifically Subpart B, in order to determine the appropriate local, state and federal requirements for disposal.

>> /Proposed methods of disposal should be used on statutory requirements of the state where disposal is to occur. The usual methods would be expected to include:/ 1) Absorbing in vermiculite, dry sand, earth, or a similar material and disposing in a secured sanitary landfill. 2) Atomizing in a suitable combustion chamber.

14. Transport Information

DOT

tert-Butyl acetate
3
UN Pack Group: II
Reportable Quantity of 5000 lb or 2270 kg

IATA

tert-Butyl acetate
3,
UN Pack Group: II

15. Regulatory Information

Clean Water Act Requirements:

The Clean Water Act (CWA) of 1972 establishes the basic structure for regulating discharges of pollutants into the waters of the United States and regulating quality standards for surface waters. Under CWA, the U.S. Environmental Protection Agency (EPA) developed the Toxic Pollutant List (40 CFR Part 401.15) and the Priority Pollutant List (40 CFR Part 423, Appendix A). These lists are to be used by EPA and States to develop the Effluent Guidelines regulations and ensure water quality criteria and standards.

>> tert-Butyl acetate is designated as a hazardous substance under section 311(b)(2)(A) of the Federal Water Pollution Control Act and further regulated by the Clean Water Act Amendments of 1977 and 1978. These regulations apply to discharges of this substance. This designation includes any isomers and hydrates, as well as any solutions and mixtures containing this substance.

TSCA Requirements:

This section provides information on requirements concerning this chemical under the Toxic Substances Control Act (TSCA) of 1976. TSCA provides EPA with authority to require reporting, record-keeping and testing requirements, and restrictions relating to chemical substances and/or mixtures. Certain substances are generally excluded from TSCA, including, among others, food, drugs, cosmetics and pesticides.

>> Section 8(a) of TSCA requires manufacturers of this chemical substance to report preliminary assessment information concerned with production, exposure, and use to EPA as cited in the preamble in 51 FR 41329. Effective date 1/26/94; Reporting date: 3/28/94.

Regulatory Information

The Australian Inventory of Industrial Chemicals

>> Chemical: Acetic acid, 1,1-dimethylethyl ester

REACH Registered Substance

>> Status: Active Update: 05-10-2021 https://echa.europa.eu/registration-dossier/-/registered-dossier/10192

>> Status: Active Update: 14-09-2020 https://echa.europa.eu/registration-dossier/-/registered-dossier/31636

New Zealand EPA Inventory of Chemical Status

>> Acetic acid, 1,1-dimethylethyl ester: HSNO Approval: HSR001094 Approved with controls

16. Other Information

Toxic Combustion Products:

Toxic products (e.g., gases and vapors) produced from the combustion of this chemical.

>> Toxic gases and vapors (such as carbon monoxide) may be released in a fire involving tert-butyl acetate.

Other Safety Information

Chemical Assessment

>> IMAP assessments - Acetate esters (C2-C4): Human health tier II assessment