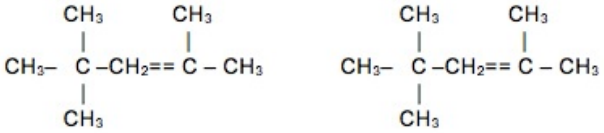
WORKPLACE ENVIRONMENTAL EXPOSURE LEVEL®

OARS WEEL

Diisobutylene (2016)

I. IDENTIFICATION

Chemical Name: An isomeric mixture of: 2,4,4-trimethyl-1-pentene (or alpha diisobutylene) and 2,4,4-trimethyl-2-pentene (or beta-diisobutylene) in an approximate ratio of 4:1, respectively. Approximately 50-100 ppm of an antioxidant (BHT) may be added.
Synonyms: Diisobutylene; diisobutene
CAS Number: 107-39-1 (alpha-diisobutylene); 107-40-4 (beta-diisobutylene); 25167-70-8 (mixed isomers)
Molecular Formula: C_8H_{16}
Structural Formula: (alpha and beta, respectively)



II. CHEMICAL AND PHYSICAL PROPERTIES[1–3]

Physical State: Clear colorless liquid
Odor Description and Threshold: Gasoline- or turpentine-like; threshold data not available.
Molecular Weight: 112.22
Conversion Factors: 1 ppm = 4.59 mg/m^3; 1 mg/m^3 = 0.22 ppm
Melting Point: -101 °C (-214 °F)
Boiling Point: 102 °C (216 °F)
Vapor Pressure: 23.2 mm Hg at 20 °C (68°F)
Saturated Vapor Concentration: ≈ 30,500 ppm
Octanol/Water Partition Coefficient: No data available
Vapor Density: 3.9
Flammability Limits in Air: LEL: 1.0%; UEL: 7.0%
Flash Point (closed cup): -9 °C (16°F)
Autoignition Temperature: 374 °C (705 °F)
Specific Gravity: 0.715 at 20 °C (68 °F)
Stability: Stable
Reactivity and Incompatibilities: Oxidizing materials can cause a vigorous reaction. Atmospheric oxygen can cause discoloration.

III. USES[4,5]

Used as a raw material for detergent intermediates, rubber tackifiers, antioxidants, lube oil additives, and organic intermediates. Diisobutylene is used to alkylate other materials. It is also used in improving coatability in paper.

IV. ANIMAL TOXICOLOGY DATA

(Specific test material is identified where that information is available)

A. Acute Toxicity

1. Lethality Data

Species	Route	LD_{50}
Rat*	Oral	>3200 mg/kg[6]
Mouse*	Oral	>3200 mg/kg[6]
Guinea Pig	Oral	>10,000 mg/kg[7]

* Alpha isomer administered undiluted; 14- day observation period

2. Eye Irritation

Very slight irritation of the conjunctiva of rabbits in both unwashed and washed eyes. Eyes appeared normal at 24 hr post-exposure. (One drop of alpha isomer administered undiluted; observations initially, and at 1, 24, and 48 hr and 14 days post-exposure.)[6]

3. Skin Absorption

Doses of the undiluted alpha isomer as high as 20 mL/kg were nonlethal by skin absorption when applied to guinea pigs under an occluded patch (14-day observation period).[6]

4. Skin Irritation

Strong irritation was noted in guinea pigs following occluded contact for 24 hr; heavy scarring and complete alopecia were noted over the entire patch area at 2 weeks post-exposure (alpha isomer).[6] A slight to moderate response has been reported in rabbits.[7]

Patches containing undiluted test material were applied to 201 human subjects. Some individuals reported a burning sensation; no irritation was observed the following day.[8]

5. Skin Sensitization

Low potential for sensitization in a guinea pig test involving topical occluded application for induction and challenge without the use of an adjuvant.[8]

6. Inhalation Toxicity

No mortality occurred in a group of 3 rats inhaling a calculated airborne concentration of approximately 32,000 mg/m^3 (7000 ppm) for 6 hr.[6] A calculated concentration of approximately 360,000 mg/m^3 (78,000 ppm as combination of vapor and aerosol) was lethal to all rats (3/3) in 5 to 9 min. Testing was conducted with the alpha isomer and animals were observed over a 14-day period.

B. Subacute Toxicity

Daily doses of 0.1 mL undiluted test material (~288 mg/kg body weight) were administered by gavage to a group of 10 rats for 10 days.[8] All animals survived to scheduled sacrifice, which was 4 days after the final treatment. There was no gross pathology noted at necropsy, and aside from slight variations in the nuclei of liver cells in a single rat, no abnormal histopathology was noted.

C. Subchronic Toxicity

No data available.

D. Chronic Toxicity/Carcinogenicity

No data available.

E. Reproductive/Developmental Toxicity

No data available.

F. Genotoxicity/Mutagenicity

Salmonella typhimurium TA100 with S-9: No activity (alpha isomer).[9] This finding was reported in a study in which diisobutylene was investigated as an impurity of trichloroethylene. The results were represented in the report as a figure showing activity approximately equal to that of the control rate at all dose levels tested.

G. Metabolism/Pharmacokinetics

Although chemical-specific data are not available, data for other octenes, including 1-octene, indicate that metabolism generally proceeds via oxidation by the cytochrome P-450 dependent mixed function oxidases; the resulting epoxides are subsequently hydrolyzed to glycols.[10,11]

V. HUMAN USE AND EXPERIENCE

Exposure to high airborne concentrations of trimethylpentenes have been reported to cause headache, inability to maintain sustained attention, vertigo, nausea, central nervous system depression, and upper respiratory tract irritation.[12] The exposure concentrations at which these effects occur have not been reported in the literature. Ingestion may cause abdominal pain and vomiting.[13]

VI. RATIONALE

No significant new literature was located since the last revision (2000) that would require a change to the recommended WEEL value. Acute toxicity data indicates a relatively low toxicity by the oral, dermal and inhalation routes of exposure. Eye irritation is reported to be slight whereas skin irritation is reported to be strong in guinea pigs causing heavy scarring and complete hair loss at the site of contact. Studies using rabbits reported slight to moderate skin irritation. Human subjects were tested and following an application of Diisobutylene to the skin a burning sensation was initially reported, but no irritation was observed the day following exposure. Acute inhalation studies in rats reported no mortality after they inhaled 7000 ppm for 6 hours. Rats inhaling 78,000 ppm as a combination of vapor and aerosol produced death in 5-9 minutes in all three rats tested.

Other published studies with exposure to Diisobutylene were a negative gavage study (~288 mg/kg body weight) following daily dosing and a negative Salmonella typhimurium TA100 study using only the alpha isomer of diisobutylene.

Human inhalation exposure to a mixture of alpha and beta Diisobutylene caused headache, inability to maintain attention, vertigo, nausea, central nervous system depression and upper respiratory irritation. The report did not quantify the concentration, but called it “high.”

For the purpose of setting an occupational exposure limit, Diisobutylene may be compared to 1-Octene. Diisobutylene and 1-Octene have the same molecular formula and similar toxicity. They both have a low order of acute toxicity from inhalation, dermal contact and ingestion. Following inhalation exposure to Diisobutylene, rats showed no mortality after breathing 7000 ppm for six hours. 1-Octene showed a threshold of mortality in an LC_{50} study at 6050 ppm for 4 hours. Eye irritation was judged minimal to very slight for either chemical. Skin irritation studies using the same species,

rabbits, reported slight to moderate irritation. A 10-day gavage study in rats with Diisobutylene at a concentration of 288 mg/kg found no gross pathology at necropsy. A gavage study using rats and a concentration of 500 mg/kg 1-Octene produced kidney and liver weight increases after 13 weeks of exposure. Unfortunately, the next lower dose of 1-octene in the study was 50 mg/kg where there were no effects. The WEEL for 1-octene is 75 ppm, based on a no observable adverse effect level (NOAEL) established in this subchronic gavage study in addition to the similarity of acute and repeat-dose toxicities of C6-C10 compounds in the olefin series.[14]

The human effects following inhalation exposure to either of these compounds is irritation of the respiratory tract, headache, nausea, and central nervous system depression. Unfortunately, at what concentration these effects are noted in humans has not been quantified. Generally speaking, branching increases the toxicity of C6 to C18 alkenes.[13] However, the available data suggest that the toxicities of Diisobutylene and 1-Octene are similar.

The rationale for this WEEL is based on analogy to 1-octene in consideration of similarity in chemical structure and mammalian toxicity. Additional support for this analogy is provided by similar toxicity of the C6-C10 compounds in the olefin series, as cited in the documentation for 1-octene. Insufficient data are available to provide a basis for the determination of a short-term exposure level (STEL).

VII. RECOMMENDED WEEL GUIDE

8-hr time-weighted average (TWA): 75 ppm (344 mg/m^3)

This WEEL value was originally established in 1996 and updated in 2000. No significant new literature was identified since the last revision (2000) that supports a change to the recommended WEEL value.

VIII. REFERENCES

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(4) Chemical Process and Production Incorporated. *Technical Bulletin and Safety Information: Diisobutylene.*; Texas City, TX.

(5) Richardson, M.; Gangolli, S. In *The Dictionary of Substances and their Effects*; Royal Society of Chemistry: Cambridge, UK, 1994; pp. 516–517.

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(9) Henschler, D.; Eder, E.; Neudecker, T.; Metzler, M. Carcinogenicity of Trichloroethylene: Fact or Artifact? *Arch. Toxicol.* **1977**, *37*, 233–236.

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(14) AIHA. *Workplace Environmental Exposure Level (WEEL) Guide Documentation for 1-Octene.*; American Industrial Hygiene Association (AIHA): Fairfax, VA, 1998.