



Recommendation from the Scientific Expert Group on Occupational Exposure Limits for pentane, isopentane and neopentane

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|---------------------------|---|------------------------------------|
| 8 hour TWA | : | 1000 ppm (3000 mg/m ³) |
| STEL (15 mins) | : | - |
| Additional classification | : | - |

Substance:

| | pentane | isopentane | neopentane |
|-------------------------------------|--------------------------------|--------------------------------|----------------------|
| | <chem>CH3-(CH2)3-CH3</chem> | <chem>(CH3)2-CH-CH2-CH3</chem> | <chem>C(CH3)4</chem> |
| Synonyms : | n-pentane | 2-methylbutane | 2,2-dimethylpropane |
| EINECS N° : | 203-692-4 | - | - |
| EEC N° : | 601-006-00-1 | 601-006-00-1 | - |
| Classification : | | | |
| CAS N° : | 109-66-0 | 78-78-4 | 590-35-2 |
| MWt : | 72.15 | 72.15 | 72.15 |
| Conversion factor (20°C, 101 kPa) : | 3.00 mg/m ³ = 1 ppm | | |



1. Occurrence/use

Pentane is a colourless liquid at room temperature, with an odour similar to that of petrol. It has a MPt of -129.7 °C, a BPt of 36.1 °C and a vapour pressure of 68.3 kPa at 25°C. The vapour density is 2.49 times that of air and it is explosive in the range 1.42 to 7.8 % in air.

Isopentane is also a colourless liquid at room temperature. It has a MPt of -19.8 °C, a BPt of 27.9 °C and a vapour pressure of 91.7 kPa at 25°C. The vapour density is 2.49 times that of air and it is explosive in the range 1.32 to 8.3 % in air.

Neopentane is gaseous at room temperature. It has a BPt of 9.5 °C and a vapour pressure of 171 kPa at 25°C. The vapour density is 2.49 times that of air and it is explosive in the range 1.4 to 8.3 % in air.

Pentane and its isomers are components of gasolines and different volatile fractions of petroleum distillation. They are used in many synthetic processes, including the manufacture of intermediate products, blowing agents and propellants, in polymerisation reactions and as extraction solvents. The most important application is in the production of petrol.

Data for production and use in the EU are not available. As commercial products, pentane and isopentane both exist as mixtures of saturated hydrocarbons with 5,6 and 7 carbon atoms. They may be obtained as laboratory reagents with purity exceeding 99%.

2. Health Significance

Very little information is available on the toxicokinetics and toxicodynamics of pentane and no specific data relating to its isomers. In the vapour state they are absorbed by the lungs by simple diffusion (Fiserova-Bergerova and Diaz, 1986). Pulmonary retention of alkanes is determined by their solubility in blood and adipose tissue. Because pentane has a lower partition coefficient than the longer chain n-alkanes it is retained less than hexane, heptane and octane and is expected to be correspondingly less toxic. No information is available on skin penetration. Endogenous production of pentane and other alkanes occurs as a result of lipid peroxidation (Wade *et al.*, 1985). Pentane is metabolised by hydroxylation to pentanol and conjugation with glucuronic acid *in vitro* (Frommer *et al.*, 1970; Notten and Henderson, 1975).

Pentane appears to be of low acute toxicity. Exposure of mice to pure pentane vapour for 5 minutes produced no overt effects at 16,000 ppm (48,000 mg/m³), slight symptoms of anaesthesia and pulmonary irritation at 32,000 and 64,000 ppm (96,000 and 192,000 mg/m³) and deep anaesthesia and pulmonary irritation at 128,000 ppm (384,000 mg/m³) (Swann *et al.*, 1974).

The critical effects of pentane appear to be irritation of the upper respiratory tract and, at very high exposure levels, narcosis. A comparative study of neurotoxicity of pentane, hexane and heptane gave no evidence for neurotoxicity following exposure to rats of 3080 ± 270 ppm (9240 ± 810 mg/m³) n-pentane (> 99% pure) for 12 h/d, 7 d/week for 16 weeks (Takeuchi *et al.*, 1981). Frontali *et al.* (1981) also observed no evidence of neurotoxicity in male rats exposed to analytical grade pentane at 3000 ppm (9000 mg/m³) for 9h/d, 5d/week for up to 30 weeks.



Studies were conducted on vapour mixtures of 25% butane, pentane, isobutane and isopentane, primarily to investigate nephrotoxicity potential. Groups of rats were exposed to the test mixture at 44, 432 and 4437 ppm (116, 1,150 and 11,800 mg/m³) for 6h/d, 5d/week over 3 weeks (Aranyi *et al.*, 1986; Halder *et al.*, 1986). No clinical reactions were observed and no exposure-related pathological lesions or changes in body weights, organ weights or serum chemistry were found.

No information is available on mutagenicity, carcinogenicity or reproductive toxicology.

Human exposure to pentane at 5000 ppm (15,000 mg/m³) for 10 minutes did not produce any symptoms (Patty and Yant, 1929). Various published reports refer to the occurrence of polyneuritis in workers exposed to mixtures of pentane and hexane (Inoue *et al.*, 1970; Gaultier *et al.*, 1973; Abbritti, 1976). In view of the absence of neurotoxicity in animal studies on pentane, and the differences in metabolism between pentane and the alkanes that are known to be neurotoxic, pentane is not thought to be responsible for the neurotoxic effects observed on exposure to such mixtures. There are no data available relating to occupation exposure to pure pentane.

Recommendation

The database on the experimental and occupational toxicology of pentane and its isomers is extremely weak, but indicates that these substances are of low toxicity with no evidence of neurotoxicity. There are no human studies available that provide a basis for deriving occupational exposure limits. Taking into account the animal studies of Takeuchi *et al.* (1981) and Frontali *et al.* (1981) showing no effects in rats exposed to pure pentane at about 3000 ppm (9000 mg/m³), and of Aranyi *et al.* (1986) and Halder *et al.* (1986) showing no effect in rats exposed to a mixture of alkanes at 4437 ppm (11,800 mg/m³) containing 25% pentane and 25% isopentane, it was considered that an 8-hour TWA of 1000 ppm (3000 mg/m³) would be adequate to allow for the uncertainties in the database and afford worker protection.

No STEL or "skin" notation was considered to be necessary.

At the levels recommended, no measurement difficulties are foreseen.



Key Bibliography

- Abbritti, G., Sicacus, A. A., Cianchetti, C., Coli, C. A., Curradi, F., Fertoni, G. F. and de Rosa, F. (1976). Shoe-makers polyneuropathy in Italy. The aetiological problem. *Br. J. Ind. Med.* **33**, 92-99.
- Anon (1995). Occupational Exposure Limits: Criteria Document for pentane, isopentane and neopentane.
- Aranyi, C., O'Shea, W. J., Halder, C. A., Holdsworth, Ch. E. and Cockrell, B. Y. (1986). Absence of hydrocarbon induced nephropathy in rats exposed subchronically to volatile hydrocarbon mixtures pertinent to gasoline. *Toxicol. Ind. Health* **2**, 85-94.
- Fiserova-Bergerova, V. and Diaz Maria, L. (1986). Determination and prediction of tissue-gas partition coefficients. *Int. Arch. Occup. Environ. Health*, **58**, 75-87.
- Frommer, U. Ullrich, V. and Staudinger, H (1970). Hydroxylation of aliphatic compounds by liver microsomes, II. Effect of phenobarbital induction in rats on specific activity and cytochrome P-450 substrate binding spectra. *Hoppe-Seyler's Z. Physiol. Chem.* **351**, 913-918.
- Frontali, N., Amantini, M. C., Spagnolo, A., Guarcini, A. M., Saltari, M. C. and Brugnone, F. (1981). Experimental neurotoxicity and urinary metabolites of the C5-C7 aliphatic hydrocarbons used as glue solvents in shoe manufacture. *Clin. Toxicol.* **18**, 1357-1367.
- Gaultier, M., Rancurel, G., Piva, C. and Efthymioc, M. L. (1973). Polyneuritis and aliphatic hydrocarbons. *J. Eur. Toxicol.* **6**, 294-296.
- Halder, C. A., van Gorp, G. S., Hatoum, N. S. and Warne, T. M. (1986). Gasoline vapor exposures. Part II. Evaluation of the nephrotoxicity of the major C4-C5 hydrocarbon components. *Am. Ind. Hyg. Assoc. J.* **47**, 173-175.
- Notten, R. F. and Henderson, P. T. (1975). Action of alkanes on drug-metabolizing enzymes from guinea-pig liver. *Biochem. Pharmacol.* **24**, 1093.
- Inoue, T., Takeuchi, Y., Takeuchi, S., Yamada, S., Suzuki, H., Matshita, T., Hiyagaki, H., Maeda, K., Matsumoto, T. (1970). Industrial health survey of high incidence of n-hexane intoxication among vinyl sandal manufacturers. *Jpn. J. Ind. Health*, **12**, 73-84.
- Patty, F. A. and Yant, W. P. (1929). Report of investigations odor intensity and symptoms produced by commercial propane, butane, pentane, hexane and heptane vapor, No. 2979, U.S. Dept. Of Commerce, Bureau of Mines.
- Swann, H. E., Kwon, B. K., Hogan, G. K., Snellings, W. M. (1974). Acute inhalation toxicology of volatile hydrocarbons. *J. Am. Ind. Hyg. Assoc.* **35**, 511.
- Takeuchi, Y., Ono, Y., Hisanaga, N., Kitoh, J., Sugiura, Y. (1980). A comparative study on the neurotoxicity of n-pentane, n-hexane and n-heptane in the rat. *Br. J. Ind. Med.* **37**, 241-247.