

The SCOEL recommendation document covers the following substances:

Substance name	EC number	CAS RN
Pentyl acetate	211-047-3	628-63-7
1-Methylbutyl acetate (2-Pentyl acetate)	210-946-8	626-38-0
3-Pentanol, acetate (8CI)(9CI) (3-Pentyl acetate)	-	620-11-1
Isopentyl acetate	204-662-3	123-92-2
2-Butanol, 2-methyl-, acetate (Tert-amyl acetate)	809-420-6	625-16-1

This text is not part of the official SCOEL Recommendation and is provided to give additional helpful information to the reader as regards chemicals addressed by the SCOEL Recommendation. The list is non-exhaustive and is presented for information purposes only.

*Recommendation from Scientific Expert Group
on Occupational Exposure Limits
for Pentyl Acetate and its Isomers*

8 hour TWA	:	50 ppm (270 mg/m ³)
STEL (15 mins)	:	100 ppm (540 mg/m ³)
Additional classification	:	-

Substance identification:

- Pentyl acetate
Synonyms : 1-amyl acetate, n-amyl acetate, 1-pentyl acetate
CH3COOC5H11
EINECS N° : 211-047-3
EEC N° : 607-130-00-2 Classification: R10
CAS N° : 628-63-7

- 2-Pentyl acetate
Synonyms : sec-amyl acetate, 2-acetoxypentane, 1-methylbutylacetate
CH3COOCH(CH3)C3H7
EINECS N° : -
EEC N° : -
CAS N° : 626-38-0

- 3-Pentyl acetate
Synonyms : 3-amyl acetate



EINECS N° : -

EEC N° : -

CAS N° : 620-11-1

- Iso-pentyl acetate

Synonyms : Iso-amyl acetate



EINECS N° : -

EEC N° : -

CAS N° : 123-92-2

- Tert-amyl acetate

Synonyms : -



EINECS N° : -

EEC N° : -

CAS N° : 625-16-1

MWt : 130.19

Conversion factor (20°C, 101kPa) : $5.41 \text{ mg/m}^3 = 1 \text{ ppm}$

Occurrence/use:

Pentyl acetates are clear, flammable liquids with characteristic fruity odours. Depending upon the structure, the MPts are between -70.8 and -78.5°C, and the BPts are between 124 and 149°C. Some of the pentyl acetates are naturally occurring compounds. 1-Pentyl acetate has been identified in various fruit (e.g. as a constituent of the volatile aroma of banana oil). Iso-pentyl acetate occurs as a pheromone in the bark beetle.

In general, pentyl acetates are produced by esterification of the corresponding alcohol with acetic acid. Pentyl acetates - mainly 1-pentyl and 2-pentyl acetate - are used as solvents in lacquers and paints, artificial leather, cellulose, celluloid, printing compounds and in smaller quantities in a range of other products such as furniture polish and nail enamels.

Technical grade pentyl acetate is a mixture of isomers.

Health Significance:

The SEG discussed the document on pentyl acetate and its isomers, prepared by the Dutch Expert Committee for Occupational Standards. Much of the available data relates to work carried out twenty years or more ago. There is a lack of data on the effects of long term exposure in humans and for animal studies on the effects of exposure at lower levels. These data gaps were partly overcome by an additional updating literature search and re-evaluation performed by a member of the SEG.

Taking into account the new data together with the Dutch Criteria Document, the SEG concluded that:

- all isomers of pentyl acetate have similar toxicologic properties,
- they are readily absorbed via the lungs,
- they are hydrolysed (like other acetates) in the body tissues into acetic acid and the corresponding pentyl-alcohols, which are then further biotransformed,
- the potential for bioaccumulation is expected to be low, although no extensive studies have been found in the literature,
- pentyl acetates show low acute toxicity with reported LCLo values > 5000 ppm,
- with these and higher exposure levels, narcotic effects are the primary systemic

effects in different species,

- at levels of 1850 ppm (10000 mg/m³) for 2h/day over 120 days, metabolic imbalance of the liver has been recorded in rabbits,
- irritation of the mucous membranes of the upper respiratory tract and of the eyes is the first response to exposure to pentyl acetate vapour and should be regarded as the critical effect; the RD50 value (mice) for pentyl acetate is estimated to be about 1500 ppm (8115 mg/m³),
- in view of the dermal LD50 value (> 20 ml/kg) for rabbits, this route of exposure is of minor importance,
- the possibility that pentyl acetate is a marginal skin sensitizer cannot be ruled out; the single report on this effect needs to be confirmed.

Reports on the toxicological effects of pentyl acetate in man relate only to short term exposure. The most sensitive short term effect of 1-pentyl acetate is initial irritation of the larynx and cough, followed by irritation of the conjunctiva and increased nasal secretion. These effects are reported to occur at 185 ppm (1000 mg/m³) within an exposure time of 30 mins, and their severity is reported to increase with the level of exposure. The available data show that irritation of the eye and the upper respiratory tract has to be regarded as the key effect/organ, at least for short term exposure. As regards systemic effects, these are considered to occur only at exposure levels which are well above the irritating concentration. The liver has been identified as one systemic target organ in subchronic animal experiments.

In general, the available data concerning effects at levels of exposure likely to occur at the workplace are very limited.

Recommendation:

On the basis of the irritant properties of pentyl acetate in man reported by von Oettingen and the RD50 investigations on mice by Alarie, the SEG recommends an 8-hour TWA exposure limit of 50 ppm (270 mg/m³), supported by a STEL (15 mins) of 100 ppm (540 mg/m³). The 8-hour TWA is well below the reported irritative effects during short term exposure and is in accordance with the range 15-150 ppm (81-810 mg/m³) indicated for the limit value from RD50 investigations.

At the level recommended, no measurement difficulties are foreseen.

Further data on the effects of long-term exposure and on actual exposure levels are considered to be necessary to confirm the recommended limit values.

Bibliography

Alarie, Y. (1981): Dose response analysis in animal studies: prediction of human responses. *Environ. Health Perspect.* 42, 9-13.

Butterworth, K.R., Gaunt, I.F., Heading, C.E., Grasso, P. and Gangolli, S.D. (1978): Short-term toxicity of n-amyl alcohol in rats. *Food.Cosmet.Toxicol.* 16, 203-207.

Divincenzo, G.D. and Krasavage, W. (1974): Serum Ornithine carbamyl-transferase as a liver response test for exposure to organic solvents. *Am.Ind.Hyg.J.*, 35, 21-29.

Dutch Expert Committee for Occupational Standards (1990): Health-based recommended occupational exposure limit for Amylacetate and its isomers. (public draft)

Final report on the Safety Assessment of Amyl acetate and Isoamylacetate (1988): *Journal of the American College of Toxicology*, 7, 705.

Inserra A., Spagna C., Carobene S., Anguilletta A.: Liver function and experimental amyl

acetate intoxication. Serum colloid lability test. *Boll.Med.Chir. Catania* (1965), 33, 687-682.

Inserra A., Spagna C., Amaro A., Carobene S.: Liver function and experimental amyl acetate intoxication. Serum proteins. *Boll.Med.Chir. Catania* (1965), 33, 693-696.

Inserra A., Spagna C., Carobene S., Anguilletta A.: Liver function and experimental amyl acetate intoxication. Blood cholesterol level and serum cholinesterase and prothrombin activities. *Boll.Med.Chir. Catania* (1965), 33, 697-708.

Inserra A., Spagna C., Carobene S., Elefante E.: Electrolytes and experimental amyl acetate intoxication. Serum sodium, potassium and chloride levels. *Boll.Soc.Med.Chir. Catania* (1965), 33, 709-720.

Inserra A., Spagna C., Carobene S., Elefante E.: Electrolytes and experimental amyl acetate intoxication. Serum calcium and magnesium. *Boll.Soc.Med.Chir. Catania* (1965), 33, 721-727.

Inserra A., Spagna C., Carobene S., Anguilletta A.: Liver function and experimental amyl acetate intoxication, behavior of lipoproteins. *Folia Med. (Naples)*, (1965), 52, (9), 579-583.

Oettingen, W.P. von (1960): The aliphatic acids and their esters: toxicity and potential dangers. *Arch.Ind.Health*, 21, 28-65.