# amyl acetate (iso-, n- and sec- isomers)

| **CAS number:** | 628-63-7 (*n-*amyl *acetate*)  626-38-0 (*sec*-amyl acetate)  123-92-2 (*iso*-amyl acetate) |
| --- | --- |
| **Synonyms:** | *iso*-amyl acetate: 3-methylbutyl acetate, isopentyl acetate, isopentyl ethanoate, banana oil  *n-*amyl *acetate*: pentyl acetate, pentyl ethanoate, pear oil, amyl acetic ester, 1-pentanol acetate  *sec*-amyl acetate: pentan-2-yl acetate, 1-methylbutyl acetate, 2-pentanol acetate, sec-amyl ethanoate |
| **Chemical formula:** | C7H14O2 |
| **Structural formula:** | CH3CO2(CH2)4CH3 |

Workplace exposure standard (retained)

| TWA: | **50 ppm (266 mg/m3)** |
| --- | --- |
| STEL: | **100 ppm (532 mg/m3)** |
| Peak limitation: | **—** |
| Notations: | **—** |
| IDLH: | **1,000 ppm (10% LEL)** |
| Sampling and analysis: | The recommended value is readily quantifiable through currently available sampling and analysis techniques. |

## Recommendation and basis for workplace exposure standard

The recommendations for *iso-*, *n-*, and *sec-* isomers of amyl acetate have been grouped based on the similarities in structure and critical effects.

A TWA of 50 ppm (266 mg/m3) is recommended for *iso*-, *n*- and *sec*-amyl acetate to protect for mild irritation to the eyes and mucous membranes.

A STEL of 100 ppm (532 mg/m3) is recommended to protect for severe irritation and provide a margin of safety for acute exposures.

## Discussion and conclusions

Amyl acetates are commonly used as solvents, flavouring agents, and insecticides. Commercial supplies of these substances often consist of mixtures of various isomers. The critical effects of *n‑* and *sec-* amyl acetate exposure are irritation to the eyes and mucous membranes (DFG, 1996; ACGIH, 2001).

The recommended TWA is based on estimates from an inhalational study in mice with mixtures of amyl acetate isomers. The concentration range that elicited a 50 per cent reduction in respiration rate (RD50: 1438 to 1562 ppm) was multiplied by a factor of 0.03 (based on the established relationship between RD50 and occupational exposures) to recommend a TWA of 50 ppm (266 mg/m3)that is considered to be protective of sensory irritants. The recommended STEL is based on a human inhalational study that reported the onset of mild throat discomfort in subjects at concentrations above 100 ppm.

## Recommendation for notations

Not classified as carcinogens according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS).

Not classified as skin sensitisers or respiratory sensitisers according to the GHS.

Insufficient evidence to warrant a recommendation for a skin notation.

# Appendix

### Primary sources with reports

| Source Year set Standard |
| --- |
| SWA Year TWA: 50 ppm (270 mg/m3); STEL: 100 ppm (541 mg/m3) | |
|  |
| ACGIH 2001 TLV-TWA: 50 ppm (266 mg/m3); TLV-STEL: 100 ppm (532 mg/m3) |
| TLV-TWA and TLV-STEL recommended to protect for irritation of the eyes and mucous membranes, narcosis, hepatotoxicity and developmental effects. TWA based on relationship between RD50 and occupational exposure to sensory irritants (0.03 × RD50).  Insufficient data to recommend carcinogenicity, skin or sensitisation notations for any isomers.  Summary of data:  Human data:   * Symptoms following inhalation include headache, fatigue, lacrimation, excessive salivation, vague nervousness, and irritation to mucous membranes, eyes, throat and nose (concentrations not specified) * Eye irritation at 300 ppm, severe throat irritation at 200 ppm, slight throat discomfort at 100 ppm (no further information provided) * Reported irritation to eyes and photophobia in exposed workers (duration 1 mo–30 yr) * Irritant effects essentially the same for all isomers but slightly less for *sec-* isomer due to longer pendent hydrocarbon chain * No adverse reaction to mixture of 20% *iso*- and 20% *n*- in repeat insult patch test (n=211; co-solvent, concentration expression and duration unspecified).   Animal data:   * All isomers are irritating to the eyes, skin and respiratory tract * Defatting action on skin and prolonged exposure (duration not specified) may lead to irritation * Rats died after exposure to air saturated with isomer mixture (8 h, ~5200 ppm at 20°C)   + no rats died after exposure to the same concentration for 4 h (no further information provided) * LD50: 5–16.6 g/kg (rat, single oral dose) for *n*- and mixed isomers * LD50: 7.4 g/kg for *iso*- isomer (rabbit, oral) * LD50:>20 mL/kg for mixed isomers, covered skin penetration test (rabbit, 24 h) * Salivation, lacrimation and irregular respiration in cats exposed to 2,200 ppm for 3.5 h or 10,600 ppm for 1 h by inhalation (mixed isomers) * Narcosis in rats exposed to 5,000 ppm for 30 min by inhalation (mixed isomers) * Slight congestion of lungs observed in guinea pigs exposed to 5,000 ppm for 13.5 h * RD50: 1438–1562 ppm (mice, no further information provided) * Intraperitoneal injection of isomeric mixture caused death in 75% of male guinea pigs at 1,500 mg/kg in hepatotoxicity study   + liver is target organ, but amyl acetate isomers have low hepatotoxicity   + lipid deposition in livers identified in high-dose group (1,500 mg/kg); not observed in low-dose group (750 mg/kg) * Very few sub-chronic studies conducted; metabolism of the substances to their corresponding alcohols would present similar toxicity to the alcohols alone   + NOAEL for *n*-isomer at least 100 mg/kg/d (rats, duration not specified) * No published data on reproductive or developmental effects available * Not mutagenic based on both *in vivo* and *in vitro* studies. |
| DFG 2000 MAK: 50 ppm (270 mg/m3) |
| MAK value protects for irritant effects.  MAK consolidated for all amyl acetate isomers in 2000.  Summary of additional data:  Human data:   * Sensitivity to light, conjunctival irritation and lacrimation reported in 30 film industry workers (3,700–14,800 ppm, 4 workers exposed for at least 4–9 yr) * Irritation to respiratory system and eyes reported in chamber study with 4 subjects (185 ppm, all isomers tested individually, 5 min).   Animal data:   * Irritation threshold estimated at 200–300 ppm * NOAEL: 593 ppm in chronic exposure study (rats, inhalation, mixed isomers, 6 h/d, 11 d) * Inadequately designed carcinogenicity study (rats) with corresponding amyl alcohols suggested tumourgenicity; study unreliable due to small sample size, lack of data describing substance purity, lack of dose-dependency investigation, and inadequate statistical analysis * Ocular irritation index of 2/10 (rabbits) * Maternal toxicity NOEL: 1,000 ppm (rabbits, inhalation, *n*-isomer, 6 h/d, last 12 d of gestation) in study measured by weight loss and reduced food consumption * Developmental NOEL: 1,500 ppm (measure of toxicity unspecified) * Developmental NOEL: 500 ppm (rats, inhalation, isomeric mixture, 6 h/d, last 9 d of gestation) in study measured by foetus weight. * Maternal NOEL: 1,500 ppm as measured by incidence of bleeding skin. |
| SCOEL 1991 TWA: 50 ppm (270 mg/m3); STEL: 100 ppm (541 mg/m3) |
| No additional data |
| OARS/AIHA NA NA |
| No report |
| HCOTN NA NA |
| No report |

### Secondary source reports relied upon

| Source |  | Year | Additional information |
| --- | --- | --- | --- |
| NTP |  | 1994 | * The National Occupational Exposure Survey (1981–1983) estimated that 97,668 employees, including 32,512 female workers, in 24 industries were potentially exposed to isoamyl acetate; did not involve measurements of actual exposures. |
| US EPA |  | 2006 | * NOEL of 3,000 ppm in whole-body inhalation study (rats) as measured by change in body weight and automated motor activity. |

### Carcinogenicity — non-threshold based genotoxic carcinogens

| Is the chemical mutagenic? | No |
| --- | --- |
| **The chemical is not a non-threshold based genotoxic carcinogen.** |  |

## Notations

| Source | Notations |
| --- | --- |
| SWA | — |
| HCIS | — |
| NICNAS | NA |
| EU Annex | NA |
| ECHA | NA |
| ACGIH | — |
| DFG | — |
| SCOEL | — |
| HCOTN | NA |
| IARC | NA |
| US NIOSH | — |

NA = not applicable (a recommendation has not been made by this Agency); — = the Agency has assessed available data for this chemical but has not recommended any notations

### Skin notation assessment

| Calculation |
| --- |
| |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | **Conclusion:** |  |  |  |  |  |  |  |  |  | |  |  | Adverse effects in human case study: | no |  |  |  |  |  |  | |  |  | Dermal LD50 ≤1000 mg/kg: | yes | 3.00 |  |  |  |  |  | |  |  | Dermal repeat-dose NOAEL ≤200 mg/kg: |  |  |  |  |  |  |  | |  |  | Dermal LD50/Inhalation LD50 <10: |  |  |  |  |  |  |  | |  |  | *In vivo* dermal absorption rate >10%: |  |  |  |  |  |  |  | |  |  | Estimated dermal exposure at WES >10%: |  |  |  |  |  |  |  | |  |  |  |  | 3 | **consider assigning a skin notation** | | | | | |  |  |  |  |  |  |  |  |  |  | |

### IDLH

| Is there a suitable IDLH value available? | Yes, based on LEL |
| --- | --- |

## Additional information

| Molecular weight: | 130.19 |
| --- | --- |
| Conversion factors at 25°C and 101.3 kPa: | 1 ppm = Number mg/m3; 1 mg/m3 = Number ppm |
| This chemical is used as a pesticide: |  |
| This chemical is a biological product: |  |
| This chemical is a by-product of a process: |  |
| A biological exposure index has been recommended by these agencies: | ACGIH  DFG  SCOEL |

## Workplace exposure standard history

| Year | Standard |
| --- | --- |
| Click here to enter year |  |

## References

American Conference of Industrial Hygienists (ACGIH®) (2018) TLVs® and BEIs® with 7th Edition Documentation, CD-ROM, Single User Version. Copyright 2018. Reprinted with permission. See the [*TLVs® and BEIs® Guidelines section*](http://www.acgih.org/tlv-bei-guidelines/policies-procedures-presentations) on the ACGIH website.

Deutsche Forschungsgemeinschaft (DFG) (2000) Pentylacetat (alle Isomeren) – MAK value documentation German language edition.

Deutsche Forschungsgemeinschaft (DFG) (1996) Pentyl acetate (all isomers) – MAK value documentation.

EU Scientific Committee on Occupational Exposure Limits (SCOEL) (1991) Recommendation from the Scientific Committee on Occupational Exposure Limits for 1-Pentyl Acetate. SCOEL//SUM/3.

National Toxicology Program (NTP) (1994) Summary of Data for Chemical Selection - Isoamyl Acetate

US Environmental Protection Agency (US EPA) (2006) Inert Reassessment – Ethyl Acetate (CAS Reg. No. 141-78-6) and Amyl Acetate (CAS Reg. No. 628-63-7) – Action Memorandum

US National Institute for Occupational Safety and Health (NIOSH) (1994) Immediately dangerous to life or health concentrations – n-amyl acetate.

US National Institute for Occupational Safety and Health (NIOSH) (1994) Immediately dangerous to life or health concentrations – sec-amyl acetate.

US National Institute for Occupational Safety and Health (NIOSH) (1994) Immediately dangerous to life or health concentrations – isoamyl acetate.