# sec-hexyl acetate

| CAS number: | 108-84-9 |
| --- | --- |
| Synonyms: | 1,3-Dimethylbutyl acetate, methyl isoamyl acetate |
| Chemical formula: | C8H16O2 |
| Structural formula: | — |

Workplace exposure standard (interim)

| TWA: | 50 ppm (295 mg/m3) |
| --- | --- |
| STEL: | — |
| Peak limitation: | — |
| Notations: | — |
| IDLH: | 500 ppm |
| Sampling and analysis: The recommended value is quantifiable through available sampling and analysis techniques. | |

## Recommendation and basis for workplace exposure standard

An interim TWA of 50 ppm (295 mg/m3) is recommended to protect for irritant effects and objectionable odour and taste in exposed workers.

Given the limited data available from the primary sources, it is recommended that a review of additional sources be conducted at the next scheduled review.

## Discussion and conclusions

*sec*-Hexyl acetate is used as a solvent and fragrance ingredient.

Critical effects of exposure are eye and upper respiratory tract irritation and objectionable taste and odour at concentrations above 100 ppm. The toxicological database for the substance is very limited, but indicates low acute toxicity (HCOTN, 2002). Chronic exposure studies for animals or humans are not presented in the available source material (ACGIH, 2018; DFG, 2000; HCOTN, 2002). A volunteer study reports eye and upper respiratory tract irritation and objectionable odour and taste at 100 ppm over fifteen minute-exposures (ACGIH, 2018).

A TWA of 50 ppm is recommended in the interim as it is expected to be protective for these effects. A detailed examination of the available toxicological data is recommended during subsequent reviews of WES due to a current lack of chronic exposure data. Particularly, no mutagenicity or carcinogenicity studies were available for the current evaluation. An entry in the HCIS database was not available.

## Recommendation for notations

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

Not classified as a skin sensitiser or respiratory sensitiser according to the GHS.

There are insufficient data to recommend a skin notation.

# Appendix

### Primary sources with reports

| Source Year set Standard |
| --- |
| SWA 1991 TWA: 50 ppm (295 mg/m3) | |
|  |
| ACGIH 2001 TLV-TWA: 50 ppm (295 mg/m3) |
| TLV-TWA intended to protect for eye and upper respiratory tract irritation and objectionable taste and odour.  Summary of data:  Presentation of toxicological data is very limited. Based on a volunteer study, air concentrations of 100 ppm elicited eye and upper respiratory tract irritation, the recommended TLV-TWA is therefore expected to be protective of these effects.  Human data:   * Irritation of the eyes and upper respiratory tract and unpleasant taste and odour above 100 ppm in volunteer study (duration and frequency not specified).   Animal data:   * LC50: >4,000 ppm (rats, 4 h); saturated vapour causes narcosis, but is non-lethal over 8 h (no further details provided) * No ADME, mutagenicity or carcinogenicity data presented.   Insufficient data to assign a TLV-STEL or notations for carcinogenicity, skin absorption or sensitisation. |
| DFG 2000 Not assigned |
| Summary of additional information:  Previous MAK of 50 ppm (1958) was based on TLV-TWA at the time; but was withdrawn due to the limited toxicological data available.  Substance is presumably hydrolysed enzymatically on mucous membranes to the corresponding alcohol and carboxylic acid. 15–99% was hydrolysed after 2 h *in vitro.*  Human data:   * No quantitative dermal absorption data available * Irritating to eyes and upper respiratory tract and objectionable odour and taste at 100 ppm (n=12, 15 min).   Animal data:   * Acute toxicity is generally low by all intake routes * LD50: 6,160 mg/kg (rats, oral) * LD50: >17,200 mg/kg (rabbits, dermal) * No repeat dose, sensitisation, genotoxicity or carcinogenicity studies available for assessment   No quantitative ADME data reported.  Insufficient data to assign notations for carcinogenicity, skin absorption or sensitisation. |
| SCOEL NA NA |
| No report. |
| OARS/AIHA NA NA |
| Not assigned. |
| HCOTN 2002 TWA: 50 ppm (300 mg/m3) |
| Summary of additional data:  Existing administrative OEL of 50 ppm considered potentially too high since local irritation effects are reported at twice this value in volunteers. Toxicological database is too limited to derive a health-based OEL.  Animal data:   * Undiluted substance is non-irritating to skin at 0.01 mL (rabbits).   Insufficient data to assign a STEL or notations for carcinogenicity, skin absorption or sensitisation. |

### Secondary source reports relied upon

| Source |  | Year | Additional information |
| --- | --- | --- | --- |
| ECHA |  | 2019 | * Pre-registered substance; not yet assessed. |

### Carcinogenicity — non-threshold based genotoxic carcinogens

| Is the chemical mutagenic? | Insufficient data |
| --- | --- |
| Is the chemical carcinogenic with a mutagenic mechanism of action? | Insufficient data |
| **Insufficient data are available to determine if the chemical is a non-threshold based genotoxic carcinogen.** | |

## Notations

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

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 |
| --- |
| Insufficient data to assign a skin notation |

### IDLH

| Is there a suitable IDLH value available? | Yes |
| --- | --- |

## Additional information

| Molecular weight: | 144.21 |
| --- | --- |
| Conversion factors at 25°C and 101.3 kPa: | 1 ppm = 5.89 mg/m3; 1 mg/m3 = 0.170 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) 1,3-Dimethylbutylacetat – MAK value documentation, German language edition.

European Chemicals Agency (ECHA) (2019) 1,3-dimethylbutyl acetate – C&L Inventory.

Health Council of the Netherlands (HCOTN) (2002) sec-Hexyl acetate. Health-based Reassessment of Administrative Occupational Exposure Limits. The Hague: Health Council of the Netherlands; publication no. 2000/15OSH/048.

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