Substance Information Document

Isoamyl acetate

1. Substance identity

Name	Isoamyl acetate
Synonyms	3-Methyl-1-butanol acetate; 3-Methyl-1-butyl acetate; 3-Methylbutyl acetate; 3-Methylbutyl ethanoate; Acetic acid, 3-methylbutyl ester; Acetic acid, isopentyl ester; Amylacetic ester; Isoamyl ethanoate; Isopentyl ethanoate; Isopentyl acetate
IUPAC Name	3-methylbutyl acetate
CAS	123-92-2

2. Toxicological information

The US FDA has identified isoamyl acetate as a "respiratory toxicant" and added the compound to its list of harmful and potentially harmful constituents (HPHCs) in tobacco products.

Based on the current existing data, isoamyl acetate does not present a concern for genetic toxicity, however, no substance-specific data were identified for carcinogenicity and reproductive and developmental toxicity. Existing data do not present a concern for skin sensitization.

Humans exposed to atmospheres containing isoamyl acetate, at 1000 or 10,000 mg/m^3 for 5 minutes, experienced irritation to the trachea, nose and throat that were more marked at the higher exposure level. Atmospheres containing 5000 mg/m^3 caused initial irritation of the mucous membranes in the throat, coughing, increased nasal secretion, dryness of the throat, and conjunctival irritation. Nasal irritation was also reported in dogs at atmospheres containing 27,000 mg/m^3 isoamyl acetate and in cats exposed to 21,000 mg/m^3, which also displayed eye irritation. Two cats exposed to atmospheres containing 1900 mL/m^3 [ppm] isoamyl acetate for 6 hours/day, for 6 days had oedema in the lungs and pneumonia.

Dizziness, disturbed vision, pain and stiffness in his jaw, difficulty swallowing, pupil constriction, excess salivation, sweating, nausea rash on the face and trunk were reported in a single case (male soldier) that was exposed 30 minutes to isoamyl acetate by inhalation (unknown concentration). For an unspecified number of humans that were exposed to atmospheres containing 5000 mg/m^3 isoamyl acetate for 30 minutes, headache and weakness were reported.

In an acute toxicity study in mouse, 1040 mL/m^3 [ppm] was determined as RD_{50} for inhalation. An LD_{50} value of 57 mmol/kg bw [7400 mg/kg bw] and an ND_{50} value of 32 mmol/kg bw [4200 mg/kg bw] were reported for rabbits after isoamyl acetate intake by oral gavage. Repeated-dose toxicity studies in rats determined 500 mg/kg bw/day and 36.5 mg/kg bw/day as NOELs.

8-hour time-weighted average (TWA) occupational exposure limits (OELs) have been established for isoamy9l acetate: from 270 mg/m^3 (50 ppm) (ACGIH, DFG, MAK and EC) to 525 mg/m^3 (100 ppm) (OSHA and NIOSH). Oral acceptable daily intake (ADI) of 3 mg/kg bw was set by JECFA.

JECFA	WHO_TRS_868.pdf
FEMA	3. GRAS Substances(2001-3124)_0.pdf (femaflavor.org)
EFSA	-
ECHA – REACH dossier	Registration Dossier - ECHA (europa.eu)
PUBCHEM	Hazardous Substances Data Bank (HSDB) : 1818 - PubChem (nih.gov)
CIR	Final Report on the Safety Assesment of Anyl Acetate and Isoamyl Acetate
OSHA	-

3. Addictiveness and attractiveness

As a flavouring agent known to impart a banana-like flavour, it might (depending on the concentration used) increase the attractiveness of an ENDS product containing it.

Dizziness and disturbed vision were reported in one man exposed to an unspecified concentration of isoamyl acetate by inhalation, and headache and weakness were reported in a number of volunteers exposed to 5000 mg/m^3 for 30 minutes. “Light narcosis; delayed death due to pneumonia” were reported in an unspecified number of cats exposed to atmospheres containing 38,000 mg/m^3 isoamyl acetate for up to 24 hours. Drowsiness was reported in an unspecified number of dogs exposed to atmospheres containing 27,000 mg/m^3 isoamyl acetate for 1 hour.

SCENIHR	-
EMA	-
PUBMED	Fassett DW and Irish DD (ed.) (1963). Patty's Industrial Hygiene and Toxicology. 2nd Edition. Vol II. Chapter XL. Fassett DW: Organic acids and related compounds. p1783. Interscience Publishers, New York (cited in Clayton and Clayton, 1982) Aliphatic alcohols and alkyl esters: narcotic and lethal potencies to tadpoles and to rabbits - PubMed (nih.gov) Severe extrapyramidal syndrome after exposition to isoamyl acetate vapour - PubMed (nih.gov)