Substance Information Document

Isoamyl hexanoate

1. Substance identity

Name	Isoamyl hexanoate
Synonyms	Isopentyl hexanoate 3-Methylbutyl hexanoate Isoamyl caproate Hexanoic acid, 3-methylbutyl ester
IUPAC Name	3-methylbutyl hexanoate
CAS	2198-61-0

2. Toxicological information

Isoamyl hexanoate was assessed in the BlueScreen assay and found negative for genotoxicity, with and without metabolic activation. There are no studies assessing the mutagenic/clastogenic activity of isoamyl hexanoate, however, read across made to isoamyl butyrate, isoamyl alcohol and hexanoic acid do not present a concern for genotoxic potential and this can be extended to isoamyl hexanoate. Therefore, based on the current existing data and use levels, isoamyl hexanoate does not present a concern for genetic toxicity.

Isoamyl hexanoate does not present a concern for skin sensitization.

There are no repeated dose toxicity data on isoamyl hexanoate. Isoamyl hexanoate will hydrolyze readily into isoamyl alcohol (CAS 123-51-3) and hexanoic acid (CAS142-62-1). Metabolite, isoamyl alcohol has sufficient repeated dose toxicity data. In an OECD 422 combined repeated dose reproduction/developmental toxicity screening test with isoamyl alcohol by oral gavage the NOAEL was determined to be 100 mg/kg/day, based on reduced body weight gain in males. In an OECD/ GLP 408 study (90 day treatment) with isoamyl alcohol, via drinking water, the NOAEL was determined to be 1600 ppm or 1250 mg/kg/day, the highest dose tested.

There are no developmental toxicity data on isoamyl hexanoate, but metabolite, isoamyl alcohol has has sufficient developmental toxicity data. In an OECD 414 developmental toxicity study conducted on female pregnant rabbits with isoamyl alcohol via inhalation, the NOAEL for developmental toxicity was determined to be 10 mg/l or 1365 mg/kg/day, the highest dose tested dose. In rats, the NOAEL for developmental toxicity after inhalation was determined to be 10 mg/l or 2695 mg/kg/day the highest dose tested. In the combined repeated dose reproduction/developmental toxicity (see above) the NOAEL was determined to be 300 mg/kg/day. Therefore, the most conservative NOAEL of 300 mg/kg/day would apply for the developmental toxicity endpoint of isoamyl hexanoate. From the same study also 300 mg/kg/ day was selected as NOAEL for reproductive toxicity.

There are no inhalation data available on isoamyl hexanoate. Based on the *Creme RIFM* model, the inhalation exposure is 0.0070 mg/day. This exposure is 200 times lower than the Cramer Class I TTC

value of 1.4 mg/day (based on human lung weight of 650 g); therefore, the exposure at the current level of use is deemed safe.

JECFA	WHO_TRS_868.pdf;jsessionid=69D19049BAE09C69530516C8447806CE
FEMA	3. GRAS Substances(2001-3124)_0.pdf (femaflavor.org)
EFSA	Scientific Opinion on the safety and efficacy of branched-chain primary aliphatic alcohols/aldehydes/acids, acetals and esters with esters containing branched-chain alcohols and acetals containing branched-chain aldehydes (chemical group 2) when used as flavourings for all animal species - - 2012 - EFSA Journal - Wiley Online Library
ECHA – REACH dossier	Pre-registered : Substance Information - ECHA (europa.eu)
PUBCHEM	3-Methylbutyl hexanoate | C11H22O2 - PubChem (nih.gov)
CIR	
OSHA	

3. Addictiveness and attractiveness

Odor Description is fruity and could be therefore attractive. No studies are available.

SCENIHR	
EMA	
PUBMED	