Substance Information Document

Ally hexanoate

1. Substance identity

Name	Ally hexanoate
Synonyms	
IUPAC Name	prop-2-en-1-yl hexanoate
CAS	123-68-2

2. Toxicological information

Allyl esters are rapidly hydrolyzed in vivo to yield allyl alcohol and the corresponding carboxylic acid (hexanoic acid for allyl hexanoate). Allyl alcohol is oxidized to acrolein, which is primarily detoxified via glutathione conjugation, but at high levels is associated with hepatotoxicity. Under the conditions of use as flavoring agent, this situation is very unlikely to happen.

The acute toxicity of allyl hexanoate has been evaluated in various studies that cover the oral (similar to OECD TG 401) and dermal (similar to OECD TG 402) routes. LD 50 values were established at 218 mg/kg bw for oral and 820 mg/kg bw for dermal, respectively, which classified this substance for acute toxicity hazard category 3 for both endpoints. No acute inhalation study has been performed on this substance, but one study (no guideline is followed) was identified on its structural analogue, allyl alcohol (CAS no. 107-18-6). LC 50 value has been determined as 0.297 mg/L. These data have been considered as the worst-case approach since allyl alcohol is more toxic than allyl hexanoate via the inhalation route.

Skin and eye irritating potential of allyl hexanoate was evaluated in OECD TG 439 and TG 405, respectively. Results indicated that this substance is not irritating to skin or eye. No skin sensitization study has been identified but based on the results (OECD TG 406) on allyl heptanoate (CAS no. 142-19-8), allyl hexanoate is not considered to be a skin sensitizer.

Both in vitro (OECD TG 471, 476, and 487) and in vivo (OECD TG 475 and TG 477) genotoxicity studies showed negative results which indicate that allyl hexanoate is not genotoxic.

Oral repeated exposure of rats to allyl hexanoate in food at a concentration of 2500 ppm (214 mg/kg bw/day) over a period of one year had no adverse effects on male and female rats, which indicated the NO(A)EL is > 214 mg/kg bw/day. No repeated inhalation or dermal study is available.

Evaluation of reproductive toxicity of allyl hexanoate was based on its read across analogue, allyl heptanoate (CAS no. 142-19-8). In an OECD TG 421 feeding study, allyl heptanoate induced some macroscopic changes in the urinary bladder (males) or in the liver and spleen (females) of the parental rats (NOEL 10 mg/kg bw/day), but no test item-related influence was noted at any of the tested doses on the growth and development of the offspring (NOEL > 100 mg/kg bw/day). Another OECD 414 study (oral gavage) was identified with allyl alcohol (CAS no. 107-18-6) in rats. No teratogenic effects were seen in this study, but dose-related increases in post-implantation loss were observed in females. The maternal LOAEL is 10 mg/kg bw/day (based on mortalities, clinical signs, food consumption and body weight gain reduction plus macroscopic liver effects seen at higher dosages) and the developmental NOAEL is 10 mg/kg bw/day.

No substance-specific carcinogenicity data were identified.

JECFA	WHO_TRS_868.pdf;jsessionid=044FEEE52AEE655177F13F5451B7E2C1
FEMA	ALLYL HEXANOATE | FEMA (femaflavor.org)
EFSA	-
ECHA – REACH dossier	Registration Dossier - ECHA (europa.eu)
PUBCHEM	Allyl hexanoate | C9H16O2 - PubChem (nih.gov)
CIR	-
OSHA	-

3. Addictiveness and attractiveness

No substance specific data were identified.

SCENIHR	-
EMA	-
PUBMED	-