Substance Information Document

Hexyl acetate

1. Substance identity

Name	Hexyl acetate
Synonyms	Acetic acid, hexyl ester; Hexyl ethanoate; Hexyl alcohol, acetate
IUPAC Name	hexyl acetate
CAS	142-92-7

2. Toxicological information

According to a RIFM Expert Panel, "based on the current existing data, hexyl acetate does not present a concern for genotoxicity". Carcinogenicity data were neither identified in human nor in non-human, and (Q)SAR assessment resulted in negative (non-carcinogenic).

RIFM noted that there were insufficient inhalation data available on hexyl acetate and therefore based their risk assessment on data for a read-across analogue, n-butyl acetate (CASRN 123-86-7). From a 13-week whole-body inhalation study in Sprague Dawley rats a NOAEC for n-butyl acetate of 2375 mg/m^3 was determined.

No skin irritation was observed when hexyl acetate (at 4% in petrolatum) was applied on human skin in a 48-hour closed patch test, whereas a human eye irritation threshold for hexyl acetate vapour was reported as 100 ppm [590mg/m^3]. Dermal LD_{50} in rabbits was reported to exceed 5000 mg/kg bw.

In oral acute toxicological studies in rats, a LD_{50} value was reported as 6160 mg hexyl acetate/kg bw, indicating a very low order of acute oral toxicity. In a rat repeated-dose toxicity study, NOAELs of 300 and 1000 mg/kg bw/day were derived or males and female, respectively. No cardiopulmonary effects were detected when rats were administered hexyl acetate at up to 1000 mg/kg bw/day by oral gavage for 13weeks.

RIFM derived a margin of exposure (MOE) for hexyl acetate of 757033 (i.e., [90844 mg/kg lung weight/day]/[0.12 mg/kg lung weight/day])".

JECFA	WHO Technical Report Series 884 910. Esters/aliphatic acyclic prim. alcohols/aliphatic linear saturated carb. acids (WHO Food Additives Series 40) (inchem.org)
FEMA	3. GRAS Substances(2001-3124)_0.pdf (femaflavor.org)
EFSA	Scientific Opinion on the safety and efficacy of straight-chain primary aliphatic alcohols/aldehydes/acids, acetals and esters with esters containing saturated alcohols and acetals containing saturated

	aldehydes (chemical group 1) when used as flavourings for all animal species - - 2013 - EFSA Journal - Wiley Online Library
ECHA – REACH dossier	Registration Dossier - ECHA (europa.eu)
PUBCHEM	Hexyl acetate | C8H16O2 - PubChem (nih.gov)
CIR	-
OSHA	-

3. Addictiveness and attractiveness

In an investigation into the most common flavouring ingredients added to e-liquids on the Dutch market, hexyl acetate (reportedly providing sweet, fruity, pear-apple,green, bananantes)was identified in 10.3% of e-liquid samples and within several flavour categories. The investigators noted that such flavourings increase e-cigarette attractiveness and use and thereby exposure to potentially toxic ingredients.

SCENIHR	-
EMA	-
PUBMED	tobaccocontrol-2019-055447.pdf (nih.gov)