Substance Information Document

Ethyl hexanoate

1. Substance identity

Name	Ethyl hexanoate
Synonyms	Ethyl caproate Hexanoic acid, ethyl ester
IUPAC Name	ethyl hexanoate
CAS	123-66-0

2. Toxicological information

Ethyl hexanoate has a low acute toxicity and repeated-dose toxicity following inhalation, oral or dermal treatment in laboratory animals and humans. The oral LD50 value was determined to be >5000 mg/kg bw in rats, and a dermal LD50 value of >5000 mg/kg bw was reported in rabbits, indicating a very low order of acute oral and dermal toxicity. Following inhalation, the systemic NOAEC19 was reported as 1331 mg/m^3 in Sprague-Dawley rats exposed to butyl propionate for 6 hours/day, 5 days/week, at concentrations of 3994 and 7987 mg/m^3. The NOAEL21 for systemic toxicity after oral gavage of ethyl hexanoate at doses of 0, 100, 300 or 1000 mg/kg bw/day in Sprague-Dawley rats (12 rats/sex/group) was reported as 1000 mg/kg bw/day.

No evidence of genotoxic activity was seen in bacteria or cultured mammalian cells. No in vivo genotoxicity or carcinogenicity data were identified.

Available data do not suggest that Ethyl hexanoate is toxic to reproduction or development. The NOAEL for reproductive toxicity was reported as 1000 mg/kg bw/day in Sprague-Dawley rats.

Regarding local effects, ethyl hexanoate is described as a respiratory irritant by Vardavas et al. (2017), as cited by NICNAS (2019) in its review of health concerns from ENDS, but no supporting data are given by NICNAS or in the paper itself. Covered contact for 48 hours with ethyl hexanoate at 4% in petrolatum was not irritating to the skin of 19 subjects, while the application of neat ethyl hexanoate to the intact or abraded skin of rabbits under an occluded patch for 24 hours was “moderately irritating”. RIFM expert panel concluded that, based on the existing data and the read-across substance methyl octanoate (CAS RN 111-11-5), ethyl hexanoate is considered a weak skin sensitiser with a defined NESIL12 of 4700 µg/cm^2. In addition, based on the available UV/Vis spectra (no significant absorption between 290 and 700 nm), the RIFM also concluded that ethyl hexanoate is not expected to present a concern for photoallergenicity.

JECFA	WHO_TRS_868.pdf;jsessionid=82B170DA92C3F40D0B615A7AA78297DD
FEMA	3. GRAS Substances(2001-3124)_0.pdf (femaflavor.org)
EFSA	-

ECHA – REACH dossier	Registration Dossier - ECHA (europa.eu)
PUBCHEM	Ethyl hexanoate | C8H16O2 - PubChem (nih.gov)
CIR	-
OSHA	-

3. Addictiveness and attractiveness

No substance-specific addictiveness data were identified.

In an investigation into the most common flavouring ingredients added to e-liquids on the Dutch market, ethyl hexanoate (reportedly providing a fruity flavour) was identified in 14% of e-liquid samples. The investigators noted that such flavourings increase e-cigarette attractiveness and use and thereby exposure to potentially toxic ingredients.

SCENIHR	-
EMA	-
PUBMED	Comprehensive overview of common e-liquid ingredients and how they can be used to predict an e-liquid's flavour category - PubMed (nih.gov)