

Compound	Octanoic acid	Data collection sheet (1/1)
N°CAS 124-07-2	CLP: H314: Skin corr. 1C	
1 ppm = 5.93 mg/m³		
Organisation name	REACH Registrants	
Risk value name	DNEL (inhalation, systemic, long-term, general population)	
Risk value (µg/m³)	No DNELs derived	
Risk value (ppb)		
Reference period		
Year	2011, updated 2018	
Key study		
Study type		
Species		
Duration of exposure in key study		
Critical effect	No hazards via inhalation identified	
Critical dose value		
Adjusted critical dose		
Single assessment factors (see table R.8.6)		
Other effects		
Confidence		

Compound	Octanoic acid (caprylic acid) C8H16O2		Factsheet
Parameter	Note	Comments	Value / descriptor
EU-LCI value and status			
EU-LCI value	1	Mass/volume [$\mu\text{g}/\text{m}^3$]	2100
EU-LCI status	2	Draft/final	Final
EU-LCI year of issue	3	Year when the EU-LCI value has been issued	2018
General information			
CLP-INDEX-No.	4	INDEX	607-708-00-4
EC-No.	5	EINECS – ELINCS - NLP	204-677-5
CAS-No.	6	Chemical Abstracts Service number	124-07-2
Harmonised CLP classification	7	Human health risk related classification	Skin corr. 1C
Molar mass and conversion factor	8	[g/mol] and [ppm – mg/m^3]	144.21 1 ppm = 5.93 mg/m^3
Key data / database			
Key study, author(s), year	9	Critical study with lowest relevant effect level	-
Read across compound	10	Where applicable	Acetic acid CAS 64-19-7 Propionic acid CAS 79-09-4
Species	11	Rat, human, etc.	-
Route/type of study	12	Inhalation, oral feed, ...	-
Study length	13	Days, subchronic, chronic	-
Exposure duration	14	Hrs/day, days/week	-
Critical endpoint	15	Effect(s), site of	-
Point of departure (POD)	16	LOAEC*L, NOAEC*L, NOEC*L, Benchmark dose, etc.	-
POD value	17	[mg/m^3] or [ppm] or [$\text{mg}/\text{kg}_{\text{BW}} \times \text{d}$]	0.5 ppm
Assessment factors (AF)			
Adjustment for exposure duration	19	Study exposure hrs/day, days/week	-
Study length	20	sa \rightarrow sc \rightarrow c (R8-5)	-
Route-to-route extrapolation	21		-
Dose-response	22 a	Reliability of dose-response, LOAEL \rightarrow NOAEL	-
	22 b	Severity of effect (R 8-6d)	-
Interspecies differences	23 a	Allometric Metabolic rate (R8-3)	-
	23 b	Kinetic + dynamic	-
Intraspecies differences	24	Kinetic + dynamic Worker - general population	-
Sensitive population	25	Children or other sensitive groups	-
Other adjustment factors Quality of whole database	26	Completeness and consistency Reliability of alternative data (R8-6 d,e)	-

Result			
Summary of assessment factors	27	Total Assessment Factor (TAF)	-
POD/TAF	28	Calculated value ($\mu\text{g}/\text{m}^3$ and ppb)	-
Molar adjustment factor	29	Used in read-across	Not applicable
Rounded value	30	$[\mu\text{g}/\text{m}^3]$	2100
Additional comments	31		
Rationale section	32		
<p>Octanoic acid (caprylic acid) is part of the volatilome of healthy humans and emitted from faeces, breath, skin and milk. It also occurs naturally in food (milk). It is used to produce esters used in perfumes and to manufacture dyes.</p> <p>The acute toxicity in rats is low; no mortality was seen after oral doses up to 2000 mg/kg. Octanoic acid was found to be a skin and eye irritant in OECD Guideline tests with rabbits (ECHA Registration dossier, 2018). There was no indication of a skin sensitisation potential in the local lymph node assay (Basketter <i>et al</i> 1988, cited in the ECHA Registration Dossier, 2018).</p> <p>The only repeated dose study available is a subchronic study where rats were given octanoic acid via their food for 84 days at doses up to 25%, corresponding to 12500 mg/kg/day. No treatment-related effects were seen. Octanoic acid showed no signs of genotoxic effects in bacterial and mammalian mutation tests and chromosomal aberration tests, with and without metabolic activation. There was no indication of reproductive toxicity in oral gavage doses up to 1000 mg/kg/day in an OECD Guideline screening test with rats (ECHA Registration Dossier, 2018).</p> <p>The adverse effect of concern is irritation. No studies addressing irritation or sensory irritation from inhalation exposure were found. However, for sensory irritation there is only a slight trend of increased potency from formic acid (C1) to butyric acid (C4) (Nielsen <i>et al</i> 2007). The EU-LCI value for n-heptanoic acid (C7) is therefore derived by read-across using the EU-LCI for propionic (C3) acid of 500 ppb (0.5 ppm, the same value was derived for acetic acid) as the point of departure. The cut-off rule of maximum two extra carbons applies; thus the conversion factor of pentanoic acid (C5) is used and the resulting EU-LCI is $(4.20 \times 500 =) 2100 \mu\text{g}/\text{m}^3$.</p> <p>According to Devos <i>et al</i> (1990), the odour threshold is $24 \mu\text{g}/\text{m}^3$ and therefore much lower than the EU-LCI value.</p> <p>References: Devos <i>et al</i> (1990): <i>Standardized Human Olfactory thresholds</i>. Oxford University press 1990 ECHA Registration dossier (2018) https://echa.europa.eu/de/registration-dossier/-/registered-dossier/15370/ (last retrieved on 4.12.2019). Nielsen GD, Wolkoff P, Alarie Y (2007) <i>Sensory irritation: Risk assessment approaches</i>. Reg Toxicol Pharmacol 48: 6-18.</p>			