Compound	Hexanoic acid	*Data collection sheet (1/1)*
N°CAS 142-62-1	**CLP:** not harmonised	
1 ppm = 4.78 mg/m³		
Organisation name	**REACH Registrants**	
Risk value name	DNEL (inhalation, systemic, long-term, general population)	
Risk value (µg/m³)	4348	
Risk value (ppb)		
Reference period		
Year	2017	
Key study	Unnamed study report, 1991	
Study type	Repeat dose 28-d oral toxicity	
Species	rat	
Duration of exposure in key study	28 d	
Critical effect	NOAEC	
Critical dose value	1000 mg/kg/d × 1/1.15 h (rat oral–>human inhalative) × 1/2 (oral absorption assumed 50% lower) = 434.8 mg/m³	
Adjusted critical dose	26.09 mg/m³	
Single assessment factors (see table R.8.6)	Dose-response 1 Duration of exposure 4 Other interspecies differences 2.5 Intraspecies 10 Quality 1 Remaining uncertainties 1 TAF 4x2.5x5=100	
Other effects	Transient breathing difficulties post-dosing. Squamous epithelial hyperplasia in forestomach.	
Confidence		

Compound	**Hexanoic acid (caproic acid)** C6H12O2		***Factsheet***
Parameter	**Note**	**Comments**	**Value / descriptor**
EU-LCI value and status			
EU-LCI value	1	Mass/volume [µg/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	-
EC-No.	5	EINECS – ELINCS - NLP	205-550-7
CAS-No.	6	Chemical Abstracts Service number	142-62-1
Harmonised CLP classification	7	Human health risk related classification	-
Molar mass and conversion factor	8	[g/mol] and [ppm – mg/m^3]	116.16 1 ppm = 4.78 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, etc.	-
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 [mg/kg$_{BW}$×d]	0.5 ppm
Assessment factors (AF)	**18**		
Adjustment for exposure duration	19	Study exposure hrs/day, days/week	-
Study length	20	sa→ sc→ c *(R8-5)*	-
Route-to-route extrapolation	21		-
Dose-response	22 a	Reliability of dose-response, LOAEL → 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 (µg/m³ and ppb)	
Molar adjustment factor	29	Used in read-across	Not applicable
Rounded value	30	[µg/m³]	2100
Additional comments	31		
Rationale section	32		

Hexanoic acid (caproic acid) is part of the human volatilome and is emitted from faeces, breath and skin. It is also used to make a variety of products: adhesives and sealants, perfumes and fragrances, cosmetics and personal care products, washing and cleaning products, air care products, biocides, plant protection products, polishes, waxes and pharmaceuticals.

Hexanoic acid has low acute toxicity; the oral LD50 in male rats is 6440 mg/kg. No animals died after up to 8 hours of inhaling saturated vapours (1.37 mg/L) (Smyth *et al* 1954, cited in ECHA registration dossier, 2018).

Rabbits dermally exposed to hexanoic acid (4 hrs, occluded) developed erythema and edema. The substance was judged corrosive to the eye based on the OECD Bovine Corneal Opacity and Permeability test in vitro (ECHA registration dossier, 2018). Ten daily dermal applications of 12% hexanoic acid caused erythema in 7 out of 10 subjects (Stillman *et al* 1975, cited in ECHA registration dossier, 2018).

Hexanoic acid was not mutagenic in a mammalian cell gene mutation assay (mouse lymphoma L5178Y cells), with or without metabolic activation (ECHA registration dossier, 2018).

There were no treatment-related adverse effects in male rats given 1000 mg/kg (highest dose tested) daily for 28 days by oral gavage, except breathing difficulties in some animals during the third week (considered non-adverse). (ECHA registration dossier, 2018).

No reproductive toxicity studies are available.

The adverse effect of concern is irritation. There are no studies that address irritation or sensory irritation from inhalation exposure. However, for sensory irritation there is only a slight trend of increased potency from formic acid (C1) to butyric acid (C4) (Nielsen *et al* 2007). The EU-LCI value for n-hexanoic acid (C4) is therefore derived by read-across using the EU-LCI value for propionic 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; the conversion factor of pentanoic acid (valeric acid) is therefore used and the resulting EU-LCI is (4.20 x 500 =) 2100 µg/m³.

This value is clearly above the odour detection threshold of 2.9 µg/m³ (Nagata 2003).

References:

ECHA registration dossier (2018) https://echa.europa.eu/de/registration-dossier/-/registered-dossier/14271/ (last retrieved on 4.12.2019).

Nagata (2003) *Measurement of odor threshold by triangle odor bag method*. https://www.env.go.jp/en/air/odor/measure/02_3_2.pdf (last retrieved on 4.12.2019).

Nielsen GD, Wolkoff P, Alarie Y (2007) *Sensory irritation: Risk assessment approaches*. Reg Toxicol Pharmacol 48: 6-18.