Compound	**n-Pentanoic acid (valeric acid)** C5H10O2		***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	607-143-00-3
EC-No.	5	EINECS – ELINCS - NLP	203-677-2
CAS-No.	6	Chemical Abstracts Service number	109-52-4
Harmonised CLP classification	7	Human health risk related classification	Skin Corr. 1B
Molar mass and conversion factor	8	[g/mol] and [ppm – mg/m^3]	102.13 1 ppm = 4.20 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		

n-Pentanoic (valeric acid) is part of the human volatilome of subjects and occurs in faeces, breath, milk and saliva. It also occurs naturally in some plants, e.g. Valeriana officinalis. It is mainly used to manufacture esters for use in perfumes and cosmetics. The acid itself has an unpleasant odour.

n-Pentanoic acid has low acute toxicity. The oral LD50 in rats is approximately 4600 mg/kg. No animals died after 6 hours of exposure to saturated vapours of the substance. Undiluted n-pentanoic acid is corrosive to rabbit skin (ECHA registration dossier, 2018).

n-Pentanoic acid was not mutagenic in the Salmonella/microsome bacterial mutagenicity assay (Ames test), with or without metabolic activation.

The only repeat dose study available is a 14 day dermal toxicity test in rabbits. The skin was treated daily with 500 mg/kg for 14 days. One female died on day 7. Decreased body weight and local skin effects (severe erythema, moderate to severe edema, necrosis, eschar formation and other skin reactions) were seen in all animals. No significant gross pathological findings were seen except for discolored gastric mucosa in some animals. Organ weights, hematological, clinical, and urinary parameters were not examined (Celanese/Hazleton, 1981 cited in ECHA registration dossier, 2018). The study did not follow valid test guidelines.

Pregnant rats were given 100, 500 or 1000 mg/kg per day of oral gavage during gestation days 6–15. No dose-related effects were seen in dams or implantations offspring at any dose, except a transient decrease in body weight at the highest dose. The study did not follow valid test guidelines. Embryotoxicity and teratogenicity were not examined (ECHA Registration dossier, 2018).

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 propionic acid (C3) (Nielsen *et al* 2007).

The EU-LCI value for n-pentanoic acid (C5) is therefore derived by read-across using the EU-LCI for propionic (C3) acid of 500 ppb (0.5 ppm, the value for acetic acid was the same) as the point of departure. The resulting EU-LCI is (4.20 x 500 =) 2100 µg/m³.

This value is clearly above the odour detection threshold of 0.16 µg/m³ (Nagata 2003).

References:

ECHA Registration dossier (2018) https://echa.europa.eu/de/registration-dossier/-/registered-dossier/14438/3/1/4. Last accessed on 10.02.2021.

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 accessed on 10.02.2021.

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