

Compound	2,2-Dimethylpropanoic acid (pivalic acid) C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>		Factsheet
Parameter	Note	Comments	Value / descriptor
<b>EU-LCI value and status</b>			
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
<b>General information</b>			
CLP-INDEX-No.	4	INDEX	-
EC-No.	5	EINECS – ELINCS - NLP	200-922-5
CAS-No.	6	Chemical Abstracts Service number	75-98-9
Harmonised CLP classification	7	Human health risk related classification	-
Molar mass and conversion factor	8	[g/mol] and [ppm – mg/m <sup>3</sup> ]	102.13 1 ppm = 4.20 mg/m <sup>3</sup>
<b>Key data / database</b>			
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 <sup>3</sup> ] or [ppm] or [mg/kg <sub>BW</sub> *d]	0.5 ppm
<b>Assessment factors (AF)</b>			
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 ( $\mu\text{g}/\text{m}^3$ 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>Pivalic acid has low acute toxicity. The oral LD50 in male rats is approximately 2000 mg/kg. No animals died after 4-hour inhalation exposure at 5.30 mg/L (ECHA Registration dossier).</p> <p>All rabbits dermally exposed to pivalic acid (4 hours, semioccluded) elicited erythema, ranging from severe to slight. Eye instillation of 0.2 mL caused severe eye irritation (ECHA registration dossier).</p> <p>n-Pivalic acid was not mutagenic in the Salmonella/microsome bacterial mutagenicity assay (Ames test), with or without metabolic activation (ECHA registration dossier).</p> <p>No adverse effects were seen in rats given 30 mg/kg daily for 28 days by oral gavage. At higher doses (100 and 300 mg/kg/day), rats were observed to sneeze and produce a dark nasal discharge, probably due to a mild irritant effect (ECHA registration dossier).</p> <p>No reproductive toxicity studies are available.</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).</p> <p>The EU-LCI value for pivalic acid (C5) is therefore derived by read-across using the EU-LCI for propionic (C3) acid of 500 ppb (0.5 ppm, for acetic acid the same value was derived) as the point of departure.</p> <p>The resulting EU-LCI is <math>(4.20 \times 500 = ) 2100 \mu\text{g}/\text{m}^3</math>.</p> <p>No data on odour detection thresholds were found.</p> <p><b>References:</b>  ECHA Registration dossier <a href="https://echa.europa.eu/de/registration-dossier/-/registered-dossier/18932/7/3/3">https://echa.europa.eu/de/registration-dossier/-/registered-dossier/18932/7/3/3</a>.  Last accessed on 10.02.2021.</p> <p>Nielsen GD, Wolkoff P, Alarie Y (2007) <i>Sensory irritation: Risk assessment approaches</i>. Reg Toxicol Pharmacol 48: 6-18.</p>			