Compound	2-Methylcyclopentanone	*Data collection sheet (1/1)*
N°CAS 1120-72-5 **1 ppm ~ 4.04 mg/m³**	**CLP: No human health classification**	
Organisation name	**AgBB (DE)**	**ANSES (FR)**
Risk value name	NIK (=LCI)	CLI (=LCI)
Risk value (mg/m³)	1.00	0.90
Risk value (ppm)	0.25	0.22
Reference period	Chronic	Chronic
Year	2018	2009
Key study	Read-across using cyclopentanone	Read-across using cyclopentanone
Study type	N/A	N/A
Species	N/A	N/A
Duration of exposure	N/A	N/A
Critical effect	N/A	N/A
Critical dose value	EU-LCI (cyclopentanone) = 900 µg/m³	OEL Denmark (cyclopentanone) = 90000 µg/m³
	NIK adopted based on EU-LCI for cyclopentanone of 900 µg/m³.	CLI adopted based on OEL Denmark of 90000 µg/m³
Adjusted critical dose		N/A
	Molecular adjustment factor of 1.17 (98.14/84.12)	N/A
Single assessment factors	N/A	Total assessment factor of 100
Other effects	N/A	N/A

Compound	**2-Methylcyclopentanone C6H10O**		***Factsheet***
Parameter	**Note**	**Comments**	**Value / descriptor**
EU-LCI value and status			
EU-LCI value	1	Mass/volume [µg/m^3]	1400
EU-LCI status	2	Draft/Final	Final
EU-LCI year of issue	3	Year when the EU-LCI value has been issued	2019
General information			
CLP-INDEX-No.	4	INDEX	N/A
EC-No.	5	EINECS – ELINCS - NLP	214-318-4
CAS-No.	6	Chemical Abstracts Service number	1120-72-5
Harmonised CLP classification	7	Human Health Risk related classification	No harmonised classification
Molar mass and conversion factor	8	[g/mol] and [ppm – mg/m^3]	98.15 g/mol 1 ppm = 4.04 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	Cyclopentanone
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/TAF in the EU-LCI fact sheet of cyclopentanone
POD value	17	[mg/m^3] or [ppm] or [mg/kg$_{BW}$×d]	1.235 mg/m^3
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 factor	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	-
AF (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 (98.15/84.12)	1.17
Rounded value	30	[µg/m³] (1235 µg/m³ x 1.17 = 1445 µg/m³)	1400
Additional comments	31		
Rationale section	32		

Data compilation and evaluation for 2-methylcyclopentanone are based on a project funded by the European Commission and carried out by Ramboll Environment & Health GmbH.

Scientific data on 2-methylcyclopentanone is limited. No assessment reports were identified in the public domain. Literature searches using PubMed, TOXNET and Google Scholar also revealed no relevant references on toxicity of 2-methylcyclopentanone. A REACH registration dossier is available for 2-methylcyclopentanone but only with limited information, as 2-methylcyclopentanone is registered for intermediate use only (ECHA, 2018).

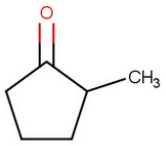
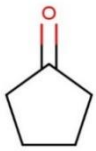
Rationale for read-across

- 2-methylcyclopentanone is a data-poor substance. No experimental animal or human data on toxicity of 2-methylcyclopentanone were identified in the public domain, making it unfeasible to derive an EU-LCI for 2-methylcyclopentanone using the *de novo* procedure.
- Cyclopentanone is considered a suitable read-across substance for 2-methylcyclopentanone with identical cyclic ring of 5 carbons and a ketone group. The sole difference is the extra methyl group (-CH_3) on 2-methylcyclopentanone. It has therefore been reported that the cyclopentanones as a group are expected to exhibit similar toxicity, as the ketone is the only functional group present on this group of cyclic hydrocarbons (Belsito et al., 2012).
- The German Committee for Health-related Evaluation of Building Products (AgBB) and the French Agency for Food, Environmental and Occupational Health and Safety (ANSES) both derived their respective LCI values (NIK for AgBB and CLI for ANSES) for 2-methylcyclopentanone by taking the read-across approach using cyclopentanone (CAS No 120-92-3). Both agencies took the occupational exposure limit (OEL) value from Denmark for cyclopentanone of 25 ppm (90 mg/m³) as the basis for the derivation (Arbejdstilsynet, 2005) and applied a default assessment factor of 100 to get 900 µg/m³ as their respective LCI value. For 2-methylcyclopentanone, the only difference between the LCI values of the two agencies is that AgBB applied a molar adjustment factor of 1.17 to get a rounded LCI value of 1000 µg/m³.
- No data could be found in the public domain on the derivation approach of the Danish OEL on cyclopentanone (25 ppm or 90 mg/m³). In particular, no further information was identified on the critical effect or point of departure (POD) for this occupational limit value, and the derivation of the EU-LCI of 2-methylcyclopentanone was performed using the ascribed EU-LCI for cyclopentanone of 900 µg/m³. Nevertheless, a subchronic inhalation rat study on cyclopentanone was identified (Elovaara et al., 1984).
- The subchronic inhalation toxicity of cyclopentanone was investigated in a study by Elovaara et al. (1984). Male Wistar rats were exposed to cyclopentanone vapour at 0, 50, 100 or 300 ppm for 6 hours/day, 5 days/week for up to 15 weeks. No significant changes in body weight were noted in any of the groups. Cyclopentanone was detected in the brain and perinatal fat starting 1 week after exposure, and levels increased in line with the exposure concentrations. Examination of liver and kidney enzymes after 15 weeks of exposure showed an increase in the kidney 7-ethoxycoumarin O-deethylase activity and a slight decrease in kidney propionaldehyde dehydrogenase activity in rats

exposed to the highest concentration of 300 ppm. Based on this study, a NOAEC of 100 ppm could be selected as the POD for kidney effects, and the following standard assessment factors would apply:

- Exposure duration: 5.6
- Study length: 2
- Interspecies difference: 2.5
- Intraspecies difference: 10

Total assessment factor: 280.

Compound	Structure	MW (g/mol)	EU- LCI value
2-Methycyclopentanone		98.15	(read-across to be used) *1400 µg/m³ or 347 ppb*
Cyclopentanone		84.12	1235 µg/m³ (unrounded *de novo* EU-LCI)

Unrounded *de novo* EU-LCI value of cyclopentanone: 1235 µg/m³ → to be used for read-across to calculate the EU-LCI of 2-methylcyclopentanone. Applying the molar adjustment factor: EU-LCI for 2-methycyclopentanone = 1235 µg/m³ x 1.17 = 1445 µg/m³ → rounded to 1400 µg/m³ (347 ppb).

No information on the odour threshold of 2-methycyclopentanone was available in the public domain.

References

Arbejdstilsynet, 2005. At-vejledning. Grænseværdier for stoffer og materialer.

Belsito D, Bickers D, Bruze M, Calow P, Dagli ML, Dekant W, Fryer AD, Greim H, Miyachi Y, Saurat JH, Sipes IG and The RIFM Expert Panel, 2012. A toxicologic and dermatologic assessment of cyclopentanones and cyclopentenones when used as fragrance ingredients. Food Chem Toxicol, 50 Suppl 3, S517-556.

ECHA 2018. 2-methylcyclopentanone. Retrieved from https://echa.europa.eu/fr/registration-dossier/-/registered-dossier/26379, last accessed on 10.02.2021.

Elovaara E, Pfaffli P and Savolainen H, 1984. Biochemical effects and decreased body burden of cyclopentanone by extended vapour inhalation. Acta Pharmacol Toxicol (Copenh), 55, 283-286.