Compound	**Other saturated aliphatic hydrocarbons C_6-C_8**	***Data collection sheet (1/4)***
See Table 1 for CAS numbers in the factsheet	See Annex 1 for existing human health-based CLP classifications in the factsheet	

Organisation name	**AgBB**	**ANSES**	**BAuA**	**ECHA**	**ECHA**
Risk value name	NIK (=LCI)	CLI (=LCI)	OEL (aliphatic C_6-C_8)	$DNEL_{(general\ population,\ long\text{-}term,\ inhalation,\ systemic)}$ [Hydrocarbons, C6-C7, n-alkanes, isoalkanes, cyclics, <5% n-hexane" (EC number: 921-024-6)]	$DNEL_{(general\ population,\ long\text{-}term,\ inhalation,\ systemic)}$ (octane & isooctane)
Risk value (µg/m³)	15000	10000	700000	608000	608000
Risk value (ppb)	N/A	N/A	N/A	N/A	~130000
Reference period	Chronic	Chronic	Chronic	Chronic	Chronic
Year	2012	1993	2017	2011, updated 2017	2011, updated in 2017
Key study	N/A	N/A	N/A	GLP-guideline study (OECD guideline 413) as reported in the registration dossier	GLP-guideline study (OECD guideline 413) as reported in the registration dossiers for octane and isooctane
Study type	N/A	N/A	N/A	Subchronic inhalation study	Subchronic inhalation study
Species	N/A	N/A	N/A	Rat	Rat
Duration of exposure	N/A	N/A	N/A	6 h/d, 5 d/wk for 13 weeks	6 h/d, 5 d/wk for 13 weeks
Critical effect	Value based on provisional OEL by the German BAuA for C_5-C_8 aliphatic hydrocarbons in 2012 (BAuA, 2012).	N/A	The group limit value is based on the 700 mg/m^3 (200 ppm) limit value for cyclohexane proposed	Subchronic toxicity or neurotoxic effects of "light alkylate naphtha distillate" (CAS 64741-66-8)	Subchronic toxicity or neurotoxic effects of "light alkylate naphtha distillate" (CAS 64741-66-8)

			by the European Commission's Scientific Committee on Occupational Exposure Limits (SCOEL).		
Critical dose value	1500 mg/m^3	N/A	N/A	NOAEC: 6646 ppm (24.3 g/m^3)	NOAEC: 6646 ppm (24.3 g/m^3)
Adjusted critical dose		N/A	N\A	N/A	N/A
Single assessment factors	100 (due to use of OEL)	N/A	None	10 (overall assessment factor)	10 (overall assessment factor)
Other effects/comments				No-threshold effect and/or no dose-response information available.	
UF_H Intraspecies variability; UF_A Interspecies variability; UF_S Used subchronic study; UF_D Data deficiencies					

Compound	**Other saturated aliphatic hydrocarbons C_6-C_8**	***Data collection sheet (2/4)***
See Table 1 for CAS numbers in the factsheet	See Annex 1 for existing CLP classifications	

Organisation name	**ACGIH**	**ACGIH**	**ACGIH**	**DFG**	**DFG**
Risk value name	TLV-TWA (hexane isomers, other than n-hexanes)	TLV-TWA (heptane, isomers)	TLV-TWA (octane, all isomers)	MAK (all hexane isomers and 2-methylcyclopentane but without n-hexane)	MAK (n-octane and isomers without trimethylpentane isomers)
Risk value (µg/m³)	1760000	1640000	1401000	1789000 (hexane isomers) 1745000 (methyl cyclopentane)	2350000
Risk value (ppb)	500000	400000	300000	500000	500000
Reference period	Chronic	Chronic	Chronic	Chronic	Chronic
Year	2001	2001	2001	2009	2004
Key study					
Study type					
Species					
Duration of exposure					
Critical effect					
Critical dose value					
Adjusted critical dose					

Single assessment factors					
Other effects/comments	A TLV-TWA of 500 ppm is recommended based on the absence of adverse effects from exposure to concentrations at or below 500 ppm.	The TLV for heptane is based on its narcotic and irritative effects, and a TLV-TWA of 400 ppm is recommended for all isomers of heptane.	On the basis of the comparison with the acute response of humans and animals to inhaled octane isomers and by analogy with other paraffinic hydrocarbons, a TLV-TWA of 300 ppm is recommended.	As written in (DFG, 2009), taking into account the MAK values for pentane isomers and n-heptane as well as data for n-hexane and studies with 2- or 3-methylpentane, the MAK value for hexane isomers (except n-hexane) and methyl cyclopentane was set at 500 mL/m^3.	MAK value derived based on structural analogies to n-heptane and n-nonane.
UF_H Intraspecies variability; UF_A Interspecies variability; UF_S Used subchronic study; UF_D Data deficiencies					

Compound	Other saturated aliphatic hydrocarbons C_6-C_8	***Data collection sheet (3/4)***
See Table 1 for CAS numbers in the factsheet	See Annex 1 for existing CLP classifications in the factsheet	

Organisation Name	**UK**	**UK**	**Sweden**	**Sweden**	**Sweden**	**Finland**
Risk value name	8 h-TWA (C_5-C_6 normal and branched chain alkanes and cycloalkanes)	8 h-TWA (≥C_7 normal and branched chain alkanes)	Level limit value (hexanes except n-hexane)	Level limit value (n-heptane and other isomers)	Level limit value (Octanes)	8h limit value (for hexanes except n-hexane)
Risk value (µg/m³)	1800000	1200000	700000	800000	900000	1800000
Risk value (ppb)	~500000 (C_6)	300000 (C_7) 210000 (C_8)	200000	200000	200000	500000
Reference period	Chronic	Chronic	Chronic	Chronic	Chronic	Chronic
Year	2011	2011	1989	1989	1989	2009
Key study	N/A	N/A	N/A	N/A	N/A	N/A
Study type						
Species						
Duration of exposure						
Critical effect						
Critical dose value	N/A	N/A	N/A	N/A	N/A	N/A
Adjusted critical dose						

Single assessment factors						
Other effects/comments	TWAs to be used for calculating OELs of mixture using the reciprocal calculation procedure (RCP)	TWAs to be used for calculating OELs of mixture using reciprocal calculation procedure (RCP)				
UF_H Intraspecies variability; UF_A Interspecies variability; UF_S Used subchronic study; UF_D Data deficiencies						

Compound	**Other saturated aliphatic hydrocarbons C_6-C_8**	***Data collection sheet (4/4)***
See Table 1 for CAS numbers in the factsheet	See Annex 1 for existing CLP classifications in the factsheet	

Organisation name	**Finland**	**Finland**	**The Netherlands**	**NIOSH**	**OSHA**
Risk value name	8h limit value (for 2-or 3-methylhexane, 2,3- or 2,4-dimethylpentane)	8h limit value (for octane, all isomers)	8-h OEL (octane)	REL-TWA (octane)	8h TWA (octane)
Risk value (µg/m³)	1200000	1400000	1450000	350000	2350000
Risk value (ppb)	300000	300000	300000	75000	500000
Reference period	Chronic	Chronic	Chronic	Chronic	Chronic
Year	2009	2009	2005	1994	1994
Key study	N/A	N/A	N/A	N/A	N/A
Study type					
Species					
Duration of exposure					
Critical effect					
Critical dose value	N/A	N/A	N/A	N/A	N/A
Adjusted critical dose					
Single assessment factors					
Other effects/comments					

UF_H Intraspecies variability; UF_A Interspecies variability; UF_S Used subchronic study; UF_D Data deficiencies

EU-LCI derivation for 'Other saturated aliphatic hydrocarbons C6-C8'

(adoption of the EU-LCI value for methylcyclopentane)

Compound	**Methylcyclopentane**		***Factsheet***
Parameter	**Note**	**Comments**	**Value / descriptor**
EU-LCI value and status			
EU-LCI value	1	Mass/volume [µg/m^3]	14000
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	Not available
EC-No.	5	EINECS – ELINCS - NLP	202-503-2
CAS-No.	6	Chemical Abstracts Service number	96-37-7
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]	84.16 1 ppm = 3.46 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	2-methylpentane CAS 107-83-5
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 EU-LCI factsheet for 2-methylpentane
POD value	17	[mg/m^3] or [ppm] or [mg/kg$_{BW}$×d]	14.707 mg/m^3 or 4.143 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 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 (84.16/86.18)	0.98
Rounded value	30	[µg/m³]	14000
Additional comments	31		
Rationale section	32		

Data compilation and evaluation for the substance group 'Other saturated aliphatic hydrocarbons C6-C8' are based on a project funded by the European Commission and carried out by Ramboll Environment & Health GmbH (formerly BiPRO GmbH).

'Other saturated aliphatic hydrocarbons (SAHs) C_6-C_8' refers to all saturated and aliphatic alkanes with six to eight carbon atoms, including branched or cyclic alkanes, except for n-hexane, cyclohexane, methylcyclohexane and n-heptane, which already have individually derived EU-LCI values due to their chemical-specific toxicity profiles. A total of 38 SAHs C_6-C_8 were identified as fitting this description.

Data compilation for this group of substances focused on SAHs C_6-C_8 that have been detected in indoor air. To determine which of the 38 substances are included in this group, an extensive literature search was conducted using various literature databases such as PubMed, Google Scholar and TOXNET, and key conference reports regarding indoor air (e.g. from the International Society of Indoor Air Quality & Climate or ISIAQ), using the CAS numbers and chemical names of the 38 SAHs C_6-C_8 as search terms. The German Association of Ecological Research Institutes (AGÖF) has also been working to assess the presence of volatile organic compounds (VOCs), including SAHs, in indoor air and to establish guidance values based on their common, average concentrations in indoor air ('statistically derived assessment'). AGÖF has published its assessment and its established guidance values for over 150 VOCs in a publicly accessible format on its website (AGÖF, 2013). The literature search revealed that 11 of the 38 SAHs C_6-C_8, namely **methylcyclopentane, 2- or 3-methylpentanes (all C_6), 2- or 3-methylhexane, 2,3- or 2,4-dimethylpentane (all C_7), octane, 2- or 3-methylheptane** and **2,2,4-trimethylpentane (isooctane) (all C_8)**, had at least two indoor air measurements. Data compilation and evaluation therefore focused primarily on these 11 SAHs.

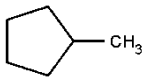
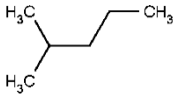
EU-LCI factsheets have been compiled for 2-methylpentane, 3-methylpentane, methylcyclopentane, the C7 substance group (2-methylhexane, 3-methylhexane, 2,3-dimethylpentane and 2,4-dimethylpentane) and the C8 substance group (octane, 2-methylheptane, 3-methylheptane and 2,2,4-trimethylpentane). The proposed EU-LCI values vary between 14000 and 20000 µg/m³ due to molar adjustment. Since these substances show similar toxicity and the studies available are of comparable quality, the EU-LCI working group decided to use a conservative approach and adopt the lowest proposed value of 14000 µg/m³ for methylcyclopentane as the EU-LCI value for the substance group 'other saturated aliphatic hydrocarbons until C8'.

Rationale for read-across

The EU-LCI derivation for methylcyclopentane was conducted using read-across from 2-methylpentane. The key assumption underlying the read-across approach using 2-methylpentane is that 2-methylpentane is the closest homologue compound of methylcyclopentane (same carbon number but in cyclic form) which has existing toxicological data and a proposed EU-LCI value (see second factsheet in this document). Both compounds show similar low systemic toxicity profiles (Chung et al., 2014; Yang et al., 2014).

Although a subchronic inhalation study of methylcyclopentane is available (performed according to OECD 413) (Yang et al., 2014), the same read-across approach was applied for all the other SAHs C_6-C_8 in order to maintain a single EU-LCI derivation approach for this group of substances. Furthermore, the key study of 2-methylpentane (subchronic inhalation exposure, also performed according to OECD 413) was considered to be the most conservative of the available subchronic inhalation studies of SAHs C_6-C_8, with the lowest NOAEC of 1160 ppm (compared to a NOAEC of 1300 ppm in the methylcyclopentane study). The EU-LCI for methylcyclopentane obtained using the read-across approach, therefore, would be lower and more conservative than the EU-LCI derived *de novo* for methylcyclopentane.

The toxicological critical endpoint for 2-methylpentane is increased relative liver weight in rats (Chung et al., 2014), which was also observed in the subchronic inhalation study for methylcyclopentane (Yang et al., 2014).

Compound	Structure	MW (g/mol)	EU-LCI value
Methylcyclopentane		84.16	Read-across to be used *14000 µg/m³*
2-methylpentane		86.18	15000 µg/m³ (*de novo* protocol) Unrounded value: 14707 µg/m³ or 4143 ppb

The unrounded EU-LCI value for 2-methylpentane is 14707 µg/m³, which was used as the read-across EU-LCI value for methylcyclopentane. There was no cut-off rule in place, as there is no difference in carbon number between the two homologue compounds.

The EU-LCI value for methylcyclopentane is 14707 µg/m³. After applying the molar adjustment factor of 0.98 at 23 °C and 1.013 atm, the rounded EU-LCI value for methylcyclopentane is 14000 µg/m³.

The proposed EU-LCI of 14000 µg/m³ (~ 4046 ppb) is above the odour detection threshold of 1700 ppb (Nagata, 2003).

References

AGÖF, 2013. AGÖF Guidance Values for Volatile Organic Compounds in Indoor Air. Available from http://www.agoef.de/orientierungswerte/agoef-voc-guidance-values.html (last retrieved on 4.12.2019).

Chung YH, Lim CH and Han JH, 2014. A study on subchronic inhalation toxicity of 2-methylpentane. Journal of Korean Society of Occupational and Environmental Hygiene, 24, 169-181.

Nagata Y, 2003. Measurement of odor threshold by triangle odor bag method. Odor Measurement Review 118, 118-127.

Yang YS, Lee SB, Choi SJ, Lee BS, Heo JD, Song CW, Kim HY, Kim JC and Lee K, 2014. Evaluation of subchronic inhalation toxicity of methylcyclopentane in rats. Food and Chemical Toxicology, 63, 186-194.

EU-LCI derivation for 2-methylpentane

Compound	**2-Methylpentane**		***Factsheet***
Parameter	**Note**	**Comments**	**Value / descriptor**
EU-LCI value and status			
EU-LCI value	1	Mass/volume [µg/m^3]	15000
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	601-007-00-7
EC-No.	5	EINECS – ELINCS - NLP	203-523-4
CAS-No.	6	Chemical Abstracts Service number	107-83-5
Harmonised CLP classification	7	Human health risk related classification	Skin irrit. 2, Asp. tox. 1, STOT SE 3
Molar mass and conversion factor	8	[g/mol] and [ppm – mg/m^3]	86.18 1 ppm = 3.55 mg/m^3
Key data / database			
Key study, author(s), year	9	Critical study with lowest relevant effect level	Chung et al., 2014
Read across compound	10	Where applicable	
Species	11	Rat, human, etc.	Rat
Route/type of study	12	Inhalation, oral feed, etc.	Inhalation
Study length	13	Days, subchronic, chronic	Subchronic
Exposure duration	14	Hrs/day, days/week	6 h/d. 5 d/wk for 13 weeks
Critical endpoint	15	Effect(s), site of	Increased relative liver and kidney weights in male rats
Point of departure (POD)	16	LOAEC*L, NOAEC*L, NOEC*L, Benchmark dose, etc.	NOAEC
POD value	17	[mg/m^3] or [ppm] or [mg/kg$_{BW}$×d]	1160 ppm
Assessment Factors (AF)	**18**		
Adjustment for exposure duration	19	Study exposure hrs/day, days/week	5.6
Study length	20	sa→ sc→ c *(R8-5)*	2
Route-to-route extrapolation factor	21		1
Dose-response	22 a	Reliability of dose-response, LOAEL → NOAEL	1
	22 b	Severity of effect *(R 8-6d)*	1
Interspecies differences	23 a	Allometric Metabolic rate *(R8-3)*	1
	23 b	Kinetic + dynamic	2.5
Intraspecies differences	24	Kinetic + dynamic Worker - general population	10
AF (sensitive population)	25	Children or other sensitive groups	1

Other adjustment factors Quality of whole database	26	Completeness and consistency Reliability of alternative data *(R8-6 d,e)*	1
Result			
Summary of assessment factors	27	Total Assessment Factor (TAF)	280
POD/TAF	28	Calculated value (µg/m³ and ppb)	14707 µg/m³ and 4143 ppb
Molar adjustment factor	29	Used in read-across	
Rounded value	30	[µg/m³]	15000
Additional comments	31		
The study was written in Korean and published in a Korean journal, but the abstract and the data in tables and figures were published in English.			
Rationale section	32		

'Other saturated aliphatic hydrocarbons (SAHs) C_6-C_8' refers to all saturated and aliphatic alkanes with six to eight carbon atoms, including branched or cyclic alkanes, except for n-hexane, cyclohexane, methylcyclohexane and n-heptane, which already have individually derived EU-LCIs due to their chemical-specific toxicity profiles. A total of 38 SAHs C_6-C_8 were identified as fitting this description.

Data compilation for this group of substances focused on SAHs C_6-C_8 that have been detected in indoor air. To determine which of the 38 substances are included in this group, an extensive literature search was conducted using various literature databases such as PubMed, Google Scholar and TOXNET, and key conference reports regarding indoor air (e.g. from the International Society of Indoor Air Quality & Climate or ISIAQ) using the CAS numbers and chemical names of the 38 SAHs C_6-C_8 as search terms. The German Association of Ecological Research Institutes (AGÖF) has also been working to assess the presence of volatile organic compounds (VOCs), including SAHs, in indoor air and to establish guidance values based on their common, average concentrations in indoor air ('statistically derived assessment'). AGÖF has published its assessments and established guidance values for over 150 VOCs in a publicly accessible format on its website (AGÖF, 2013). The literature search revealed that 11 of the 38 SAHs C_6-C_8, namely **methylcyclopentane, 2- or 3-methylpentanes (all C_6), 2- or 3-methylhexane, 2,3- or 2,4-dimethylpentane (all C_7), octane, 2- or 3-methylheptane** and **2,2,4-trimethylpentane (isooctane) (all C_8)**, had at least two indoor air measurements. Data compilation and evaluation therefore focused primarily on these 11 SAHs.

Data sources for the EU-LCI derivation of other SAHs C_6-C_8 include assessment reports on SAHs published by organisations or authorities (ACGIH, 2001a, 2001b, 2001c; ATSDR, 1999; DFG, 2009, 2014; Goldhaber et al., 2007; OECD, 2010). In particular, there is a 2014 report from a project commissioned by the German Institute for Occupational Safety and Health of the German Social Accident Insurance (IFA) that provides an extensive review of the toxicological data on hydrocarbon solvent mixtures, covering specifically C_6, C_7 and C_8 aliphatic hydrocarbon solvents (FoBIG, 2014), and a comprehensive review of the toxicity of hydrocarbon solvents including SAHs published in 2015 (McKee et al., 2015). Only the information relevant for this group of substances was reviewed and considered for the EU-LCI derivation.

Rationale for key study/POD

No chronic inhalation studies of the 11 targeted SAHs C_6-C_8 were identified, but studies were identified of repeated inhalation exposure to methylcyclopentane, 2-methylpentane, 3-methylpentane, n-octane and 2,2,4-trimethylpentane (single substance exposure). These studies consistently showed low systemic toxicity (reversible lethargy, mild indications of intoxication, slight increase in serum markers or organ weight) and no mortality upon exposure to SAHs C_6-C_8 at concentrations up to ~6000 ppm (Sung et al., 2010; Lammers et al., 2011; Chung et al., 2014; Yang et al., 2014; Chung et al., 2016; ECHA, 2017b).

It is important to clarify that in the absence of n-hexane, other SAHs C_6-C_8 do not trigger neurotoxicity such as peripheral neuropathy. Peripheral neuropathy is only attributable to exposure to n-hexane, due to its specific metabolism to 2,5-hexanedione, a toxic gamma diketone metabolite (Egan et al., 1980; Frontali et al., 1981; Ono et al., 1981; Galvin & Bond, 1999a; Galvin & Bond, 1999b). Additionally, kidney effects (such as renal accumulation of alpha-2µ-globulin leading to nephropathy) found in male rats after exposure to

certain SAHs such as 2,2,4-trimethylpentane are not considered relevant for human risk assessment due to the species-specific and sex-specific effect.

There are, however, two subchronic studies with a reported chemical-specific effect of increased relative liver weight after inhalation exposure to either 2-methylpentane or methylcyclopentane in rats (Chung et al., 2014; Yang et al., 2014). Both studies were considered suitable as key studies for the EU-LCI derivation.

The subchronic inhalation study of 2-methylpentane (published in Korean, with abstract and data tables and figures provided in English) was performed in accordance with OECD test guideline 413 on groups of 10 Sprague-Dawley rats (of each sex) exposed to 0, 290, 1160 or 4640 ppm for 6 hours/day, 5 days/week for 13 weeks. No mortality or clinical symptoms were observed in any of the exposed animals. Key observed effects included a dose-dependent increase in serum total cholesterol in exposed male rats at ≥ 290 ppm and a dose-dependent increase in relative liver and kidney weights in exposed male rats (with statistical significance reached at 4640 ppm). Histopathological examination and scoring revealed altered renal effects (e.g. cystic change in renal tubules) and goblet cell hyperplasia in the nasal cavity in exposed male rats. No significant changes were observed in exposed female rats. The nasal cavity effect was considered by the authors to be a non-specific and local effect (i.e. not a systemic toxic effect), due to the nature of the study (Chung et al., 2014). As explained above, the renal effects observed in male rats are species-specific and sex-specific, and the no-observed-adverse-effect concentration (NOAEC) was set at 1160 ppm.

A subchronic inhalation study of methylcyclopentane was also performed in accordance with OECD test guideline 413 (subchronic inhalation toxicity: 90-day study) on groups of 10 Sprague-Dawley rats (of each sex) exposed to 0, 290, 1300 or 5870 ppm for 6 hours/day, 5 days/week for 13 weeks. Various observations and measurements such as clinical signs, mortality, body weight, food consumption, ophthalmoscopy, urinalysis, haematology, serum biochemistry, gross pathology, organ weights and histopathology were carried out. The observed effects were clinical symptoms such as increased salivation and rubbing against the cage wall, and increased liver weight in rats of both sexes exposed to 5870 ppm, as well as slightly higher kidney weight in female rats exposed to 5870 ppm. There were also significant increases in serum total cholesterol and phospholipid levels in exposed male rats at ≥ 290 ppm. Histopathological examination and scoring revealed no significant differences in findings such as (1) tubular degeneration/regeneration or hypertrophy/hyperplasia or inflammatory cell foci in the kidneys, (2) inflammatory cell foci, focal necrosis, hepatocyte vacuolation or bile duct hyperplasia in the liver, (3) foamy macrophages in the lung or (4) olfactory degeneration/regeneration in the nasal cavity. The NOAEC for this study was established at 1300 ppm (Yang et al., 2014).

This effect of increased relative liver weight, as observed in both these studies, was selected as the critical effect for the EU-LCI derivation. For the point of departure, the more conservative NOAEC for the same effect was selected from two subchronic inhalation studies, i.e. 1160 ppm for 2-methylpentane instead of 1300 ppm for methylcyclopentane (Chung et al., 2014). This value is also considered the most conservative observed-effect level, as the other studies reported the highest-tested concentrations as their NOAECs.

The EU-LCI derivation was performed *de novo* specifically for 2-methylpentane, which is the tested SAH in the selected key study. The EU-LCI derivation for the other selected SAHs C_6-C_8 was performed separately using the read-across approach on the basis of this key study of 2-methylpentane.

Assessment factors (AF)

Standard default assessment factors to adjust for exposure duration, study length, intraspecies and intraspecies differences were applied. The assessment factors applied are:

- adjustment for exposure duration: 5.6
- study length: 2
- interspecies difference: 2.5
- intraspecies difference: 10

The total assessment factor is 280.

This resulted in a calculated EU-LCI value of 14707 µg/m³ (taking the conversion factor of 2-methylpentane of 1 ppm = 3.55 mg/m³ at 23 °C). A derived EU-LCI for 2-methylpentane of 15000 µg/m³ is proposed.

References

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ACGIH, 2001b. American Conference of Governmental Industrial Hygienists. Hexane isomers, other than n-hexane. Documentation of the Threshold Limit Values and Biological Exposure, 9 pages.

ACGIH, 2001c. American Conference of Governmental Industrial Hygienists. Octane, all isomers. Documentation of the Threshold Limit Values and Biological Exposure, 9 pages.

AGÖF, 2013. AGÖF Guidance Values for Volatile Organic Compounds in Indoor Air. Available from http://www.agoef.de/orientierungswerte/agoef-voc-guidance-values.html (last retrieved on 4.12.2019).

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DFG, 2009. Hexan-Isomeren (außer n-Hexan) und Methylcyclopentan [MAK Value Documentation in German language, 2009]. The MAK-Collection for Occupational Health and Safety: Wiley-VCH Verlag GmbH & Co. KGaA.

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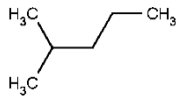
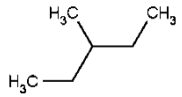
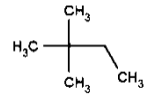
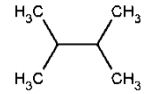
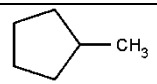
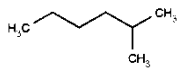
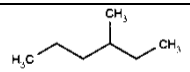
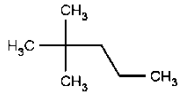
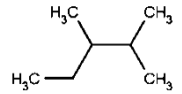
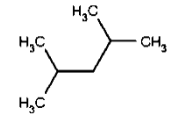
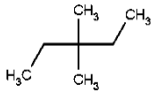
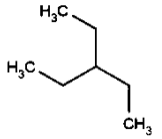
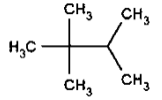
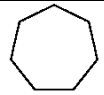
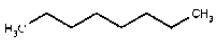
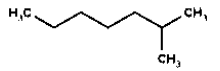
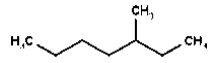
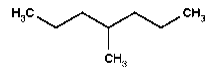
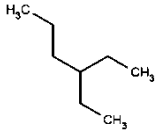
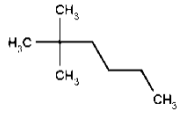
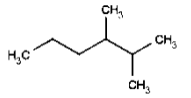
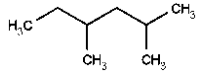
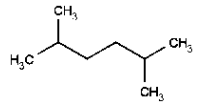
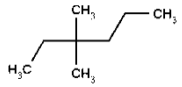
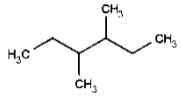
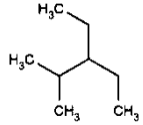
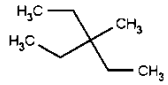
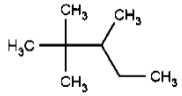
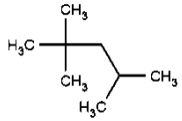
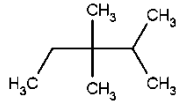
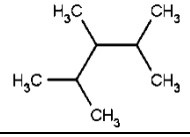
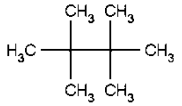
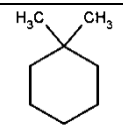
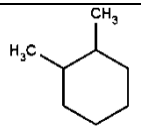
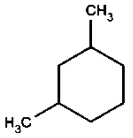
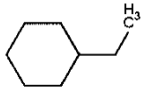
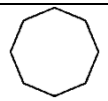
Table 1: Identity of other saturated aliphatic hydrocarbons (SAHs) C_6-C_8 (total of 38 substances)

IUPAC name	Synonyms	CLP-Index no.	EC no.	CAS no.	Sum formula	Structural formula
SAHs with 6 carbons (n = 5)						
2-Methylpentane	i-Caproylhydride, i-Hexane, isohexane	601-007-00-7	203-523-4	107-83-5	C_6H_{14}	
3-Methylpentane	Diethyl-methyl-methane	601-007-00-7	202-481-4	96-14-0	C_6H_{14}	
2,2-Dimethylbutane	Neohexane	601-007-00-7	200-906-8	75-83-2	C_6H_{14}	
2,3-Dimethylbutane	Diisopropyl	601-007-00-7	201-193-6	79-29-8	C_6H_{14}	
Methylcyclopentane	N/A	N/A	202-503-2	96-37-7	C_6H_{12}	
SAHs with 7 carbons (n = 9)						
2-Methylhexane	isoheptane ethyl-isobutyl-methane	601-008-00-2	209-730-6	591-76-4	C_7H_{16}	
3-Methylhexane	N/A	601-008-00-2	209-643-3	589-34-4	C_7H_{16}	
2,2-Dimethylpentane	neoheptane	601-008-00-2	209-680-5	590-35-2	C_7H_{16}	
2,3-Dimethylpentane	N/A	601-008-00-2	209-280-0	565-59-3	C_7H_{16}	
2,4-Dimethylpentane	N/A	601-008-00-2	203-548-0	108-08-7	C_7H_{16}	

IUPAC name	Synonyms	CLP-Index no.	EC no.	CAS no.	Sum formula	Structural formula
3,3-Dimethylpentane	N/A	601-008-00-2	209-230-8	562-49-2	C_7H_{16}	
3-Ethylpentane	N/A	601-008-00-2	210-529-0	617-78-7	C_7H_{16}	
2,2,3-Trimethylbutane	N/A	601-008-00-2	207-346-3	464-06-2	C_7H_{16}	
Cycloheptane	N/A	N/A	291-64-5	291-64-5	C_7H_{14}	
SAHs with 8 carbons (n = 24)						
Octane	N/A	601-009-00-8	203-892-1	111-65-9	C_8H_{18}	
2-Methylheptane	Isooctane	601-009-00-8	209-747-9	592-27-8	C_8H_{18}	
3-Methylheptane	N/A	601-009-00-8	209-660-6	589-81-1	C_8H_{18}	
4-Methylheptane	N/A	601-009-00-8	209-650-1	589-53-7	C_8H_{18}	
3-Ethylhexane	N/A	601-009-00-8	210-621-0	619-99-8	C_8H_{18}	
2,2-Dimethylhexane	N/A	601-009-00-8	209-689-4	590-73-8	C_8H_{18}	
2,3-Dimethylhexane	N/A	601-009-00-8	209-547-1	584-94-1	C_8H_{18}	

IUPAC name	Synonyms	CLP-Index no.	EC no.	CAS no.	Sum formula	Structural formula
2,4-Dimethylhexane	N/A	601-009-00-8	209-649-6	589-43-5	C_8H_{18}	
2,5-Dimethylhexane	N/A	601-009-00-8	209-745-8	592-13-2	C_8H_{18}	
3,3-Dimethylhexane	N/A	601-009-00-8	209-243-9	563-16-6	C_8H_{18}	
3,4-Dimethylhexane	N/A	601-009-00-8	209-504-7	583-48-2	C_8H_{18}	
3-Ethyl-2-methylpentane	N/A	601-009-00-8	210-187-2	609-26-7	C_8H_{18}	
3-Ethyl-3-methylpentane	N/A	601-009-00-8	213-923-0	1067-08-9	C_8H_{18}	
2,2,3-Trimethylpentane	N/A	601-009-00-8	209-266-4	564-02-3	C_8H_{18}	
2,2,4-Trimethylpentane	Isooctane	601-009-00-8	208-759-1	540-84-1	C_8H_{18}	
2,3,3-Trimethylpentane	N/A	601-009-00-8	209-207-2	560-21-4	C_8H_{18}	
2,3,4-Trimethylpentane	N/A	601-009-00-8	209-292-6	565-75-3	C_8H_{18}	

IUPAC name	Synonyms	CLP-Index no.	EC no.	CAS no.	Sum formula	Structural formula
2,2,3,3-Tetramethylbutane	hexamethyl-ethane	601-009-00-8	209-855-6	594-82-1	C_8H_{18}	
1,1-Dimethylcyclohexane	N/A	N/A	209-687-3	590-66-9	C_8H_{18}	
1,2-Dimethylcyclohexane	N/A	N/A	583-57-3	583-57-3	C_8H_{16}	
1,3-Dimethylcyclohexane	N/A	N/A	209-707-0	591-21-9	C_8H_{16}	
1,4-Dimethylcyclohexane	1,4-dimethyl-hexane Hexahydro-p-xylene	N/A	209-663-2	589-90-2	C_8H_{16}	
Ethylcyclohexane	N/A	N/A	1678-91-7	1678-91-7	C_8H_{16}	
Cyclooctane	N/A	N/A	206-031-8	292-64-8	C_8H_{16}	

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Annex 1: Health-based CLP classifications of other SAHs C_6-C_8

Human health-based CLP classifications for the other saturated aliphatic hydrocarbons C_6-C_8.

Name	CAS	Health-based CLP classification
SAHs with 6 carbons (n = 5)		
2-Methylpentane	107-83-5	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
3-Methylpentane	96-14-0	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,2-Dimethylbutane	75-83-2	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,3-Dimethylbutane	79-29-8	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
Methylcyclopentane	96-37-7	Asp. Tox. 1 (H304)*
SAHs with 7 carbons (n = 9)		
2-Methylhexane	591-76-4	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
3-Methylhexane	589-34-4	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,2-Dimethylpentane	590-35-2	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,3-Dimethylpentane	565-59-3	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,4-Dimethylpentane	108-08-7	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
3,3-Dimethylpentane	562-49-2	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
3-Ethylpentane	617-78-7	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,2,3-Trimethylbutane	464-06-2	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
Cycloheptane	291-64-5	Asp. Tox. 1 (H304)*
SAHs with 8 carbons (n = 24)		
Octane	111-65-9	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2-Methylheptane	592-27-8	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
3-Methylheptane	589-81-1	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
4-Methylheptane	589-53-7	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
3-Ethylhexane	619-99-8	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,2-Dimethylhexane	590-73-8	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,3-Dimethylhexane	584-94-1	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,4-Dimethylhexane	589-43-5	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,5-Dimethylhexane	592-13-2	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
3,3-Dimethylhexane	563-16-6	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
3,4-Dimethylhexane	583-48-2	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
3-Ethyl-2-methylpentane	609-26-7	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
3-Ethyl-3-methylpentane	1067-08-9	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,2,3-Trimethylpentane	564-02-3	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,2,4-Trimethylpentane	540-84-1	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,3,3-Trimethylpentane	560-21-4	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,3,4-Trimethylpentane	565-75-3	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
2,2,3,3-Tetramethylbutane	594-82-1	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
1,1-Dimethylcyclohexane	590-66-9	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
1,2-Dimethylcyclohexane	583-57-3	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
1,3-Dimethylcyclohexane	591-21-9	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
1,4-Dimethylcyclohexane	589-90-2	Skin Irrit. 2 (H315); Asp. Tox. 1 (H304); STOT SE 3 (H336)
Ethylcyclohexane	1678-91-7	Asp. Tox. 1 (H304); STOT SE 3 (H336)*
Cyclooctane	292-64-8	Asp. Tox. 1 (H304)*

* Only notified classification and labelling according to CLP criteria (i.e. not harmonised).

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