Compound	1-Propenylbenzene	*Data collection sheet*
N°CAS 637-50-3 (cis) **N°CAS 873-66-5 (trans)**	**EU- Classification:** **CLP:** Eye Irrit. 2 (H319); STOT SE 3 (H335)	
Organisation name	**AgBB**	
Risk value name	NIK ('Lowest Concentration of Interest')	
Risk value (mg/m³)	1.2	
Risk value (ppm)	-	
Reference period	Chronic (general population)	
Year	2018	
Key study	NTP (2007)	
Study type	Chronic inhalation study (0, 100, 300, 1000 ppm) with 2-phenylpropene	
Species	Rat	
Duration of exposure in key study	6 h/d, 5 d/week, 105 weeks	
Critical effect	Lesions of nasal olfactory epithelium	
Critical dose value	LOAEC (2-phenylpropene): 490 mg/m³ (100 ppm)	
Adjusted critical dose	6/24 x 5/7 => 87.5 mg/m³	
Single assessment factors (see table R.8.6)		
Other effects		
Remarks	Read-across was applied and α-methylstyrene (2-phenyl-propene) was used as test item instead of 1 phenylpropene. No molar adjustment is necessary because both compounds are structural isomers with the same molar mass.	
UF_L Used LOAEL; UF_H Intraspecies variability; UF_A interspecies variability; UF_S Used subchronic study UF_D data deficiencies		

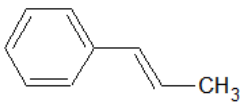
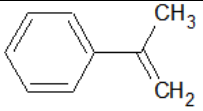
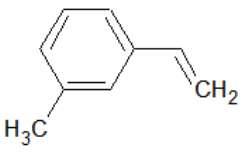
Compound	**1-Propenylbenzene (ß-methylstyrene) C9H10**		***Factsheet***
Parameter	**Note**	**Comments**	**Value / descriptor**
EU-LCI value and status			
EU-LCI value	1	Mass/volume [µg/m^3]	1200
EU-LCI status	2	Draft/Final	Final
EU-LCI year of issue	3	Year when the EU-LCI value has been issued	2019
General information			
CLP-INDEX-No.	4	INDEX	-
EC-No.	5	EINECS – ELINCS - NLP	211-287-9 (cis) 212-848-0 (trans)
CAS-No.	6	Chemical Abstracts Service number	637-50-3 (cis) 873-66-5 (trans)
Harmonised CLP classification	7	Human Health Risk related classification	
Molar mass and conversion factor	8	[g/mol] and [ppm – mg/m^3]	118.2 1 ppm = 4.9 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-phenylpropene (α-methylstyrene)
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]	POD/TAF from the fact sheet for 2-phenylpropene: 1.166 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)	1166 µg/m³ (240 ppb)
Molar adjustment factor	29	Used in read-across	1
Rounded value	30	[µg/m³]	1200
Additional comments	31		
Rationale section	32		

Data compilation and evaluation for 1-propenylbenzene is based on a project funded by the German Environment Agency (Voss, 2020).

Rationale for read-across

- Data poor compound: no adequate toxicological data for 1-propenylbenzene; *de novo* derivation of EU-LCI is not possible.
- Read-across from EU-LCI value of 2-phenylpropene (adopted in 2018): 2-phenylpropene shows structural and physicochemical similarities to 1-propenylbenzene, both compounds are isomers differing only in the position of the methyl group of the side chain.
- Toxicological critical endpoint for 2-phenylpropene: lesions of olfactory nasal epithelium.
- The key assumption underlying the read-across of the EU-LCI value from 2-phenylpropene to 1-propenylbenzene is that both compounds have the same critical endpoint (local epithelial damage) and this is due to their structural similarity. The same approach was taken when deriving a NIK value for 1-propenylbenzene by AgBB (2018). The key assumption is further strengthened by the observation that vinyl toluenes, structurally related isomers of 2- and 1-propenylbenzene with an unbranched side-chain similar to 1-propylene benzene, also lead to lesions in the nasal epithelia of rats (NTP 1990).

Compound	Structure	MW [g/mol]	EU-LCI value (µg/m³)
1-propenylbenzene (ß-methylstyrene) (trans-form)		118.2	1 200 (proposed)
2-phenylpropene (α-methylstyrene)		118.2	1 200 (final)
m-vinyl toluene (3-methylstyrene) (one of three isomers)		118.2	1 200 (final)

Data for 1-propenylbenzene (ß-methylstyrene)

1-Propenylbenzene is a pale yellow liquid with an unpleasant odour. It is a by-product in the synthesis of 2-phenylpropene (α-methylstyrene) and may be present as an impurity (up to 0.5 %) in 2-phenylpropene. 1-propenylbenzene occurs in two isomeric forms (cis and trans).

Very few data are available on the toxicity of 1-propenylbenzene. 1-propenylbenzene is metabolised with the formation of cinnamyl alcohol (Peele, 1977). Acute exposure is reported to be irritating to eyes, mucous membranes, and skin (IPCS, 2006). A comparative study of the ototoxicity of various aromatic solvents in rats revealed that trans-1-propenylbenzene does produce ototoxic effects. However, its potency is not higher than that of 2-phenylpropene and is lower than that of styrene (Gagnaire und Langlais, 2005). *In vitro* data indicate that the epoxide of trans-1-propenylbenzene induces sister chromatid exchange but not gene mutations in mammalian cells and is not mutagenic in bacteria (GESTIS, 2014). There are no further genotoxicity or other toxicity studies available. No data on the toxicity of the cis-form were identified in the available literature.

The derivation of the EU-LCI value for the read-across compound, 2-phenylpropene, is based on the lesions observed in the nasal epithelia in rats. Similar effects were also observed in mice when testing at the same concentration. Since both compounds, 1-propenylbenzene and 2-phenylpropene, are structural isomers, the molar adjustment factor is 1 leading to the same EU-LCI value of 1200 µg/m^3 for 1-propenylbenzene.

The substance is reported to have an unpleasant odour. However, no data on odour thresholds are available.

References

Gagnaire F, Langlais C (2005) Relative ototoxicity of 21 aromatic solvents. Arch Toxicol 79:346-354

GESTIS (1996) Dataset for trans-propenylbenzene. GESTIS Substance database. Online: www.dguv.de/ifa/gestis-database (last retrieved on 9.02.2021)

IPCS (2006) International Chemical Safety Card (ICSC) 0736: trans-beta-methylstyrene (CAS No. 873-66-5). Online: http://www.inchem.org/documents/icsc/icsc/eics0736.htm (last retrieved on 9.02.2021)

NTP (1990) NTP Technical Report on the Toxicology and Carcinogenesis of vinyl toluene (mixed isomers) (65%-71% meta-isomer and 32%-35% para-isomer) (CAS no. 25013-15-4) in F344/N rats and B6C3f1 mice (inhalation studies). U.S. Department of Health and Human Services PHS, National Institutes of Health: www.ntp.niehs.nih.gov/ntp/htdocs/lt_rpts/tr375.pdf (last retrieved on 9.02.2021)

Peele, J., Oswald, E. (1977) Metabolism of naturally occurring propenylbenzene derivatives: III. Allylbenzene, propenylbenzene, and related metabolic products. BBA 497, 598-607

Voss, J.-U. (2018) Toxicological basic data for the derivation of EU-LCI values for five substances from building products. UBA Texte 16/2020. https://www.umweltbundesamt.de/publikationen/toxicological-basic-data-for-the-derivation-of-eu-1 (last retrieved on 9.02.2021)