Benzenemethanamine, «alpha»-methyl-, (S)-

Other names:	(-)-«alpha»-Phenethylamine
	(R)-(+)-.alpha.-methylbenzylamine
	(R)-(+)-1-phenylethylamine
	(S)-(-)-«alpha»-Methylbenzylamine
	(S)-«alpha»-Methylbenzenemethanamine
	L(-)-«alpha»-Methylbenzylamine
	L-(-)-1-Phenylethylamine
	L-(-)-«alpha»-Phenylethylamine
	L-«alpha»-methylbenzylamine
Inchi:	InChI=1S/C8H11N/c1-7(9)8-5-3-2-4-6-8/h2-7H,9H2,1H3/t7-/m1/s1
InchiKey:	RQEUFEKYXDPUSK-SSDOTTSWSA-N
Formula:	C8H11N
SMILES:	CC(N)c1ccccc1
Mol. weight [g/mol]:	121.18
CAS:	2627-86-3

Physical Properties

Property code	Value	Unit	Source
gf	192.90	kJ/mol	Joback Method
hf	56.59	kJ/mol	Joback Method
hfus	12.19	kJ/mol	Joback Method
hvap	54.60 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.17		Crippen Method
logp	1.706		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	460.20	K	NIST Webbook
tc	709.62	K	Joback Method
tf	274.60	K	Joback Method
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	287.73	J/mol×K	671.55	Joback Method
cpg	228.83	J/mol×K	481.21	Joback Method
cpg	242.28	J/mol×K	519.28	Joback Method
cpg	254.86	J/mol×K	557.35	Joback Method
cpg	266.60	J/mol×K	595.41	Joback Method
cpg	277.54	J/mol×K	633.48	Joback Method
cpg	297.20	J/mol×K	709.62	Joback Method
rhol	965.38	kg/m3	298.15	Enthalpic changes on mixing two couples of S- and R-enantiomers of benzyl-(1-phenyl-ethyl)-amine, 1-phenylethylamine, 1-phenyl-ethanol, butyric acid oxiranylmethyl ester, 4-methyl-[1,3]dioxolan-2-one, 2-chloro-methyloxirane and 3-hydroxyisobutyric acid methyl ester at T = 298.15 K

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpic changes on mixing two couples of S- and R-enantiomers of benzyl-(1-phenyl-ethyl)-amine, 1-phenylethylamine, 1-phenyl-ethanol, butyric acid oxiranylmethyl ester, 4-methyl-[1,3]dioxolan-2-one, 2-chloro-methyloxirane and 3-hydroxyisobutyric acid methyl ester at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.10.019
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2627863&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume