Dibenzylamine, alpha-methyl, (-)-

Other names: (R)-(+)-N-benzyl-1-phenylethylamine
(S)-(-)-N-BENZYL-1-PHENETHYLAMINE
Benzenemethanamine, «alpha»-methyl-N-(phenylmethyl)-, («alpha»S)-
Benzenemethanamine, Â«alphaÂ»-methyl-N-(phenylmethyl)-, (Â«alphaÂ»S)-
N-benzyl-1-phenylethanamine #
Inchi: InChI=1S/C15H17N/c1-13(15-10-6-3-7-11-15)16-12-14-8-4-2-5-9-14/h2-11,13,16H,12H2
InchiKey: ZYZHMSJNPCYUTB-CYBMUJFWSA-N
Formula: C15H17N
SMILES: CC(NCc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 211.30
CAS: 17480-69-2

Physical Properties

Property code	Value	Unit	Source
gf	387.19	kJ/mol	Joback Method
hf	168.32	kJ/mol	Joback Method
hfus	24.26	kJ/mol	Joback Method
hvap	59.58	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.537		Crippen Method
mcvol	184.670	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
tb	645.69	K	Joback Method
tc	883.35	K	Joback Method
tf	349.31	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.81	J/mol×K	645.69	Joback Method
cpg	493.64	J/mol×K	685.30	Joback Method
cpg	510.10	J/mol×K	724.91	Joback Method
cpg	525.27	J/mol×K	764.52	Joback Method

cpg	539.24	J/mol×K	804.13	Joback Method
cpg	552.10	J/mol×K	843.74	Joback Method
cpg	563.92	J/mol×K	883.35	Joback Method
rhol	1007.70	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

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=C17480692&Units=SI
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

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