N-Benzyl-2-phenethylamine

Other names: Benzeneethanamine, N-(phenylmethyl)-
N-benzylphenethylamine
Inchi: InChI=1S/C15H17N/c1-3-7-14(8-4-1)11-12-16-13-15-9-5-2-6-10-15/h1-10,16H,11-13H2
InchiKey: UPABQMWFWCMOFV-UHFFFAOYSA-N
Formula: C15H17N
SMILES: c1ccc(CCNCc2ccccc2)cc1
Mol. weight [g/mol]: 211.30
CAS: 3647-71-0

Physical Properties

Property code	Value	Unit	Source
gf	389.63	kJ/mol	Joback Method
hf	173.60	kJ/mol	Joback Method
hfus	27.79	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.019		Crippen Method
mcvol	184.670	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
tb	646.13	K	Joback Method
tc	878.87	K	Joback Method
tf	364.31	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.35	J/mol×K	646.13	Joback Method
cpg	492.77	J/mol×K	684.92	Joback Method
cpg	508.88	J/mol×K	723.71	Joback Method
cpg	523.78	J/mol×K	762.50	Joback Method
cpg	537.53	J/mol×K	801.29	Joback Method
cpg	550.22	J/mol×K	840.08	Joback Method
cpg	561.92	J/mol×K	878.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C3647710&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume