Benzeneethanamine, N-(2-phenylethyl)-

Other names: Bis(2-phenylethyl)amine
Diphenethylamine
Inchi: InChI=1S/C16H19N/c1-3-7-15(8-4-1)11-13-17-14-12-16-9-5-2-6-10-16/h1-10,17H,11-14H
InchiKey: ACSAKRLPJQIBFB-UHFFFAOYSA-N
Formula: C16H19N
SMILES: c1ccc(CCNCCc2ccccc2)cc1
Mol. weight [g/mol]: 225.33
CAS: 6308-98-1

Physical Properties

Property code	Value	Unit	Source
gf	398.05	kJ/mol	Joback Method
hf	152.96	kJ/mol	Joback Method
hfus	30.38	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.061		Crippen Method
mcvol	198.760	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	1867.00		NIST Webbook
tb	669.01	K	Joback Method
tc	897.25	K	Joback Method
tf	375.58	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.65	J/mol×K	669.01	Joback Method
cpg	545.39	J/mol×K	707.05	Joback Method
cpg	561.84	J/mol×K	745.09	Joback Method
cpg	577.07	J/mol×K	783.13	Joback Method
cpg	591.17	J/mol×K	821.17	Joback Method
cpg	604.21	J/mol×K	859.21	Joback Method

cpg	616.28	J/mol×K	897.25	Joback Method

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=C6308981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume