1,2-Ethanediamine, N,N'-bis(phenylmethyl)-

Other names:	1,2-Bis(benzylamino)ethane
	1,2-Ethanediamine, N1,N2-bis(phenylmethyl)-
	Benzathine
	Benzatin
	DBED
	Ethylenediamine, N,N'-dibenzyl-
	N,N'-Dibenzyl-1,2-ethanediamine
	N,N'-Dibenzyl-1,2-ethylenediamine
	N,N'-Dibenzyl-ethane-1,2-diamine
	N,N'-Dibenzylethylenediamine
	N,N'-bis(phenylmethyl)ethane-1,2-diamine
	NSC 5632
	USAF DO-53
Inchi:	InChI=1S/C16H20N2/c1-3-7-15(8-4-1)13-17-11-12-18-14-16-9-5-2-6-10-16/h1-10,17-18H
InchiKey:	JUHORIMYRDESRB-UHFFFAOYSA-N
Formula:	C16H20N2
SMILES:	c1ccc(CNCCNCc2ccccc2)cc1
Mol. weight [g/mol]:	240.34
CAS:	140-28-3

Physical Properties

Property code	Value	Unit	Source
gf	487.44	kJ/mol	Joback Method
hf	206.43	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	68.63	kJ/mol	Joback Method
log10ws	-1.21		Aqueous Solubility Prediction Method
logp	2.566		Crippen Method
mcvol	208.740	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
tb	719.18	K	Joback Method
tc	945.67	K	Joback Method
tf	428.24	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.13	J/mol×K	719.18	Joback Method
cpg	599.88	J/mol×K	756.93	Joback Method
cpg	615.39	J/mol×K	794.68	Joback Method
cpg	629.74	J/mol×K	832.43	Joback Method
cpg	643.00	J/mol×K	870.18	Joback Method
cpg	655.27	J/mol×K	907.92	Joback Method
cpg	666.63	J/mol×K	945.67	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	468.20	K	0.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C140283&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume