N'-Benzyl-N,N-dimethylethylenediamine

Other names:	1,2-Ethanediamine, N,N-dimethyl-N'-(phenylmethyl)- Ethylenediamine, N'-benzyl-N,N-dimethyl- N,N-Dimethyl-N'-benzylethylenediamine N-Benzyl-N,N-dimethylenediamine 2-benzylaminoethyldimethylamine
Inchi:	InChI=1S/C11H18N2/c1-13(2)9-8-12-10-11-6-4-3-5-7-11/h3-7,12H,8-10H2,1-2H3
InchiKey:	LLSJAFHDYCTFCM-UHFFFAOYSA-N
Formula:	C11H18N2
SMILES:	CN(C)CCNCc1ccccc1
Mol. weight [g/mol]:	178.27
CAS:	103-55-9

Physical Properties

Property code	Value	Unit	Source
gf	354.32	kJ/mol	Joback Method
hf	87.16	kJ/mol	Joback Method
hfus	26.41	kJ/mol	Joback Method
hvap	50.83	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.338		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
tb	540.37	K	Joback Method
tc	740.99	K	Joback Method
tf	325.28	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.84	J/mol×K	540.37	Joback Method
cpg	402.40	J/mol×K	573.81	Joback Method
cpg	417.99	J/mol×K	607.24	Joback Method
cpg	432.66	J/mol×K	640.68	Joback Method

cpg	446.43	J/mol×K	674.12	Joback Method
cpg	459.37	J/mol×K	707.56	Joback Method
cpg	471.50	J/mol×K	740.99	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.20	K	1.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103559&Units=SI
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

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

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