Dibemethine

Other names:	Benzenemethanamine, N-methyl-N-(phenylmethyl)-
	Dibenzylamine, N-methyl-
	Dibemethin
	Dibenzylmethylamine
	DBMA
	L 566
	Methyldibenzylamine
	N-Methyl-N,N-Dibenzylamine
	N-Methyldibenzylamine
	N,N-Dibenzylmethylamine
	Revoxyl
	NSC 163900
Inchi:	InChI=1S/C15H17N/c1-16(12-14-8-4-2-5-9-14)13-15-10-6-3-7-11-15/h2-11H,12-13H2,1H
InchiKey:	WYZDCUGWXKHESN-UHFFFAOYSA-N
Formula:	C15H17N
SMILES:	CN(Cc1ccccc1)Cc1ccccc1
Mol. weight [g/mol]:	211.30
CAS:	102-05-6

Physical Properties

Property code	Value	Unit	Source
gf	411.02	kJ/mol	Joback Method
hf	187.66	kJ/mol	Joback Method
hfus	25.71	kJ/mol	Joback Method
hvap	55.58	kJ/mol	Joback Method
ie	7.85	eV	NIST Webbook
log10ws	-3.87		Crippen Method
logp	3.319		Crippen Method
mcvol	184.670	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1657.10		NIST Webbook
rinpol	1657.10		NIST Webbook
ripol	2251.00		NIST Webbook
ripol	2251.00		NIST Webbook
tb	608.40	K	Joback Method
tc	839.25	K	Joback Method
tf	344.12	K	Joback Method

vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.00	J/mol×K	608.40	Joback Method
cpg	477.58	J/mol×K	646.87	Joback Method
cpg	494.77	J/mol×K	685.35	Joback Method
cpg	510.66	J/mol×K	723.82	Joback Method
cpg	525.33	J/mol×K	762.30	Joback Method
cpg	538.86	J/mol×K	800.77	Joback Method
cpg	551.35	J/mol×K	839.25	Joback Method

Sources

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=C102056&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume