Diphenylamine, 5-chloro-2-methylamino

Other names: Clobazam, hydrolysis
Inchi: InChI=1S/C13H13ClN2/c1-15-12-8-7-10(14)9-13(12)16-11-5-3-2-4-6-11/h2-9,15-16H,1H
InchiKey: YFSSUNICRFFYOV-UHFFFAOYSA-N
Formula: C13H13ClN2
SMILES: CNc1ccc(Cl)cc1Nc1ccccc1
Mol. weight [g/mol]: 232.71

Physical Properties

Property code	Value	Unit	Source
gf	430.99	kJ/mol	Joback Method
hf	229.67	kJ/mol	Joback Method
hfus	31.13	kJ/mol	Joback Method
hvap	67.67	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	4.125		Crippen Method
mcvol	178.710	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	697.93	K	Joback Method
tc	942.42	K	Joback Method
tf	449.39	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.00	J/mol×K	697.93	Joback Method
cpg	463.01	J/mol×K	738.68	Joback Method
cpg	475.89	J/mol×K	779.43	Joback Method
cpg	487.71	J/mol×K	820.17	Joback Method
cpg	498.53	J/mol×K	860.92	Joback Method

cpg	508.42	J/mol×K	901.67	Joback Method
cpg	517.47	J/mol×K	942.42	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=R17896&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume