Norketamine

Inchi: InChI=1S/C14H16ClNO2/c1-10(17)16-14(9-5-4-8-13(14)18)11-6-2-3-7-12(11)15/h2-3,6-7
InchiKey: RRTNLABORIXPCK-UHFFFAOYSA-N
Formula: C14H16ClNO2
SMILES: CC(=O)NC1(c2ccccc2Cl)CCCCC1=O
Mol. weight [g/mol]: 265.74

Physical Properties

Property code	Value	Unit	Source
gf	14.69	kJ/mol	Joback Method
hf	-250.22	kJ/mol	Joback Method
hfus	21.61	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.814		Crippen Method
mcvol	198.860	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1889.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	780.46	K	Joback Method
tc	1039.14	K	Joback Method
tf	518.49	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.39	J/mol×K	780.46	Joback Method
cpg	583.36	J/mol×K	823.57	Joback Method
cpg	599.47	J/mol×K	866.69	Joback Method
cpg	614.90	J/mol×K	909.80	Joback Method
cpg	629.82	J/mol×K	952.91	Joback Method
cpg	644.42	J/mol×K	996.02	Joback Method
cpg	658.85	J/mol×K	1039.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R593385&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume