Ketamine

Other names:	Cyclohexanone, 2-(2-chlorophenyl)-2-(methylamino)-, (.+/-.)-
	Cyclohexanone, 2-(o-chlorophenyl)-2-(methylamino)-
	Cyclohexanone, 2-(o-chlorophenyl)-2-(methylamino)-, (.+/-.)-
	CI 581 base
	CLSTA 20
	Ketaject
	Ketalar base
	2-(o-Chlorophenyl)-2-(methylamino)cyclohexanone
	2-(Methylamino)-2-(2-chlorophenyl)cyclohexanone
	(.+/-.)-2-(O-Chlorophenyl)-2-(methylamino)cyclohexanone
	(.+/-.)-Ketamine
	dl-Ketamine
	NSC 70151
Inchi:	InChI=1S/C13H16ClNO/c1-15-13(9-5-4-8-12(13)16)10-6-2-3-7-11(10)14/h2-3,6-7,15H,4-
InchiKey:	YQEZLKZALYSWHR-UHFFFAOYSA-N
Formula:	C13H16ClNO
SMILES:	CNC1(c2ccccc2Cl)CCCCC1=O
Mol. weight [g/mol]:	237.72
CAS:	100477-72-3

Physical Properties

Property code	Value	Unit	Source
gf	135.19	kJ/mol	Joback Method
hf	-117.00	kJ/mol	Joback Method
hfus	17.42	kJ/mol	Joback Method
hvap	61.82	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.898		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1861.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1861.00		NIST Webbook
tb	703.71	K	Joback Method

tc	963.81	K	Joback Method
tf	457.29	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.62	J/mol×K	703.71	Joback Method
cpg	514.78	J/mol×K	747.06	Joback Method
cpg	531.88	J/mol×K	790.41	Joback Method
cpg	548.08	J/mol×K	833.76	Joback Method
cpg	563.57	J/mol×K	877.11	Joback Method
cpg	578.53	J/mol×K	920.46	Joback Method
cpg	593.11	J/mol×K	963.81	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100477723&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