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
	(RS)-2-(2-chlorophenyl)-2-(methylamino)cyclohexanone
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:	6740-88-1

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
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	578.53	J/mol×K	920.46	Joback Method
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	593.11	J/mol×K	963.81	Joback Method
hfust	26.60	kJ/mol	365.70	NIST Webbook

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=C6740881&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
hfust: Enthalpy of fusion at a given temperature
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume