Methoxetamine

Inchi: InChI=1S/C15H21NO2/c1-3-16-15(9-5-7-13(17)11-15)12-6-4-8-14(10-12)18-2/h4,6,8,10,
InchiKey: JUWIQHNNBJANEB-UHFFFAOYSA-N
Formula: C15H21NO2
SMILES: CCNC1(c2cccc(OC)c2)CCCC(=O)C1
Mol. weight [g/mol]: 247.33
CAS: 1239943-76-0

Physical Properties

Property code	Value	Unit	Source
gf	58.96	kJ/mol	Joback Method
hf	-274.76	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	64.29	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.643		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1929.50		NIST Webbook
rinpol	1929.50		NIST Webbook
tb	734.46	K	Joback Method
tc	977.03	K	Joback Method
tf	472.14	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.90	J/mol×K	734.46	Joback Method
cpg	624.62	J/mol×K	774.89	Joback Method
cpg	643.27	J/mol×K	815.32	Joback Method
cpg	661.00	J/mol×K	855.74	Joback Method
cpg	677.92	J/mol×K	896.17	Joback Method
cpg	694.15	J/mol×K	936.60	Joback Method
cpg	709.84	J/mol×K	977.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1239943760&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

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