Fluvoxamine (ketone)

Inchi: InChI=1S/C13H15F3O2/c1-18-9-3-2-4-12(17)10-5-7-11(8-6-10)13(14,15)16/h5-8H,2-4,9H
InchiKey: VYKSRLDHXQURKA-UHFFFAOYSA-N
Formula: C13H15F3O2
SMILES: COCCCCC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 260.25

Physical Properties

Property code	Value	Unit	Source
gf	-654.15	kJ/mol	Joback Method
hf	-928.47	kJ/mol	Joback Method
hfus	27.69	kJ/mol	Joback Method
hvap	52.88	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.705		Crippen Method
mcvol	183.020	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1525.00		NIST Webbook
tb	599.37	K	Joback Method
tc	787.79	K	Joback Method
tf	351.56	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.59	J/mol×K	599.37	Joback Method
cpg	484.82	J/mol×K	630.77	Joback Method
cpg	498.23	J/mol×K	662.18	Joback Method
cpg	510.85	J/mol×K	693.58	Joback Method
cpg	522.70	J/mol×K	724.98	Joback Method
cpg	533.81	J/mol×K	756.38	Joback Method
cpg	544.23	J/mol×K	787.79	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=R196013&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