Fluvoxamine, carboxylic acid (ketone), methylated

Inchi: InChI=1S/C13H13F3O3/c1-19-12(18)4-2-3-11(17)9-5-7-10(8-6-9)13(14,15)16/h5-8H,2-4H

InchiKey: DYQDZAIIQQXMMY-UHFFFAOYSA-N

Formula: C13H13F3O3

SMILES: COC(=O)CCCC(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 274.24

Physical Properties

Property code	Value	Unit	Source
gf	-783.07	kJ/mol	Joback Method
hf	-1041.05	kJ/mol	Joback Method
hfus	29.29	kJ/mol	Joback Method
hvap	59.62	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.231		Crippen Method
mcvol	184.590	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1550.00		NIST Webbook
rinpol	1550.00		NIST Webbook
tb	653.24	K	Joback Method
tc	848.91	K	Joback Method
tf	401.49	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.03	J/mol×K	653.24	Joback Method
cpg	501.85	J/mol×K	685.85	Joback Method
cpg	513.84	J/mol×K	718.46	Joback Method
cpg	525.03	J/mol×K	751.08	Joback Method
cpg	535.46	J/mol×K	783.69	Joback Method
cpg	545.15	J/mol×K	816.30	Joback Method
cpg	554.15	J/mol×K	848.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R195996&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