Fluvoxamine

Other names:	5-Methoxy-4'-(trifluoromethyl)valerophenone (E)-O-(2-aminoethyl)oxime
	1-Pentanone, 5-methoxy-1-(4-(trifluoromethyl)phenyl)-, O-(2-aminoethyl)oxime, (E)-
	Fluvoxamina
	61718-82-9
	1-Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl)oxime, (1E)-
	(1E)-5-methoxy-1-[4-(trifluoromethyl)phenyl]-1-pentanone, O-(2-aminoethyl)oxime
Inchi:	InChI=1S/C15H21F3N2O2/c1-21-10-3-2-4-14(20-22-11-9-19)12-5-7-13(8-6-12)15(16,17)
InchiKey:	CJOFXWAVKWHTFT-UHFFFAOYSA-N
Formula:	C15H21F3N2O2
SMILES:	COCCCCC(=NOCCN)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	318.33
CAS:	54739-18-3

Physical Properties

Property code	Value	Unit	Source
hf	-883.17	kJ/mol	Joback Method
hvap	67.03	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.201		Crippen Method
mcvol	231.160	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
tb	762.77	K	Joback Method
tc	963.48	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54739183&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

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature