Fluvoxamine, carboxylic acid, methylated, acetylated

Inchi: InChI=1S/C17H21F3N2O4/c1-12(23)21-10-11-26-22-15(4-3-5-16(24)25-2)13-6-8-14(9-7-

InchiKey: RXQJTXRHXFFNIW-PXLXIMEGSA-N

Formula: C17H21F3N2O4

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

Mol. weight [g/mol]: 374.35

Physical Properties

Property code	Value	Unit	Source
hf	-1129.93	kJ/mol	Joback Method
hvap	80.77	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.905		Crippen Method
mcvol	262.480	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinpol	2355.00		NIST Webbook
tb	893.91	K	Joback Method
tc	1103.50	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R196008&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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