Fluoxetine

Other names:	(+/-)-N-Methyl-gamma-(4-(trifluoromethyl)phenoxy)benzenepropanamine (.+/-.)-N-Methyl-3-phenyl-3-[(«alpha»,la,«alpha»-trifluoro-p-tolyl)oxy]propylamine (.+/-.)-N-Methyl-3-phenyl-3-[(«alpha»,«alpha»,«alpha»-trifluoro-p-tolyl)oxy]propylamine Benzenepropanamine, N-methyl-«gamma»-[4-(trifluoromethyl)phenoxy]- Benzenepropanamine, N-methyl-«gamma»-[4-(trifluoromethyl)phenoxy]-, (.+/-.)- N-Methyl-3-phenyl-3-[4-(trifluoromethyl)phenoxy]-1-propanamine N-methyl-3-phenyl-3-[4-(trifluoromethyl)phenoxy]propan-1-amine Prozac
Inchi:	InChI=1S/C17H18F3NO/c1-21-12-11-16(13-5-3-2-4-6-13)22-15-9-7-14(8-10-15)17(18,19
InchiKey:	RTHCYVBBDHJXIQ-UHFFFAOYSA-N
Formula:	C17H18F3NO
SMILES:	CNCCC(Oc1ccc(C(F)(F)F)cc1)c1ccccc1
Mol. weight [g/mol]:	309.33
CAS:	54910-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-292.19	kJ/mol	Joback Method
hf	-613.73	kJ/mol	Joback Method
hfus	32.07	kJ/mol	Joback Method
hvap	63.36	kJ/mol	Joback Method
log10ws	-1.59		Aqueous Solubility Prediction Method
logp	4.435		Crippen Method
mcvol	224.030	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
rinpol	1887.90		NIST Webbook
rinpol	1887.90		NIST Webbook
tb	713.43	K	Joback Method
tc	923.89	K	Joback Method
tf	453.65	K	Aqueous Solubility Prediction Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.93	J/mol×K	713.43	Joback Method
cpg	650.83	J/mol×K	748.51	Joback Method
cpg	665.57	J/mol×K	783.58	Joback Method
cpg	679.22	J/mol×K	818.66	Joback Method
cpg	691.83	J/mol×K	853.74	Joback Method
cpg	703.49	J/mol×K	888.81	Joback Method
cpg	714.26	J/mol×K	923.89	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54910893&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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