Fluacizine

Other names:	Phenothiazine, 10-diethylaminopropionyl-3-trifluoromethyl-, hydrochloride 10-Diethylaminopropionyl-3-trifluoromethyl phenothiazine hydrochloride Fluoracizine 10-[3-(Diethylamino)propionyl]-2-(trifluoromethyl)phenothiazine 10H-Phenothiazine, 10-[3-(diethylamino)-1-oxopropyl]-2-(trifluoromethyl)- Phenothiazine, 10-(N,N-diethyl-«beta»-alanyl)-2-(trifluoromethyl)- Fluoracizine base Ftoracizine 2-Trifluoromethyl-10-(3-diethylamino-propionyl)-phenothiazine Phtorazisin
Inchi:	InChI=1S/C20H21F3N2OS/c1-3-24(4-2)12-11-19(26)25-15-7-5-6-8-17(15)27-18-10-9-14
InchiKey:	VHEOUJNDDFHPGJ-UHFFFAOYSA-N
Formula:	C20H21F3N2OS
SMILES:	CCN(CC)CCC(=O)N1c2ccccc2Sc2ccc(C(F)(F)F)cc21
Mol. weight [g/mol]:	394.45
CAS:	30223-48-4

Physical Properties

Property code	Value	Unit	Source
ie	7.89 ± 0.07	eV	NIST Webbook
log10ws	-5.80		Crippen Method
logp	5.567		Crippen Method
mcvol	277.470	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30223484&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume