Trifluoperazine

Other names: 10-(3-(4-Methyl-1-piperazinyl)propyl)-2-(trifluoromethyl)phenothiazine
10-(«gamma»-(N'-Methylpiperazino)propyl)-2-trifluoromethylphenothiozine
10-(Â«gammaÂ»-(N'-Methylpiperazino)propyl)-2-trifluoromethylphenothiozine
10-[3-(4-methylpiperazin-1-yl)propyl]-2-(trifluoromethyl)phenothiazine
10H-Phenothiazine, 10-[3-(4-methyl-1-piperazinyl)propyl]-2-(trifluoromethyl)-
2-Trifluoromethyl-10-[3'-(1-methyl-4-piperazinyl)propyl]phenothiazine
Flurazine
NSC 17474
Phenothiazine, 10-[3-(4-methyl-1-piperazinyl)propyl]-2-(trifluoromethyl)-
RP 7623
TFP
Trifluoperazin
Trifluoperazina
Trifluoromethyl-10-(3'-(1-methyl-4-piperazinyl)propyl)phenothiazine
Trifluoromethylperazine
Trifluoroperazine
Trifluperazine
Triflurin
Trifluroperizine
Triperazine
Triphtazine

Inchi: InChI=1S/C21H24F3N3S/c1-25-11-13-26(14-12-25)9-4-10-27-17-5-2-3-6-19(17)28-20-8-

InchiKey: ZEWQUBUPAILYHI-UHFFFAOYSA-N

Formula: C21H24F3N3S

SMILES: CN1CCN(CCCN2c3ccccc3Sc3ccc(C(F)(F)F)cc32)CC1

Mol. weight [g/mol]: 407.50

CAS: 117-89-5

Physical Properties

Property code	Value	Unit	Source
ie	7.31 ± 0.08	eV	NIST Webbook
ie	7.43 ± 0.37	eV	NIST Webbook
ie	7.10 ± 0.07	eV	NIST Webbook
log10ws	-4.52		Aqueous Solubility Prediction Method
logp	4.946		Crippen Method
mcvol	289.110	ml/mol	McGowan Method

rinpol	2688.00	NIST Webbook
rinpol	2641.00	NIST Webbook
rinpol	2685.00	NIST Webbook
rinpol	2666.00	NIST Webbook
rinpol	2682.00	NIST Webbook
rinpol	2691.00	NIST Webbook
rinpol	2683.00	NIST Webbook
rinpol	2683.00	NIST Webbook
rinpol	2650.00	NIST Webbook
rinpol	2695.00	NIST Webbook
rinpol	2685.00	NIST Webbook
rinpol	2685.00	NIST Webbook
rinpol	2710.00	NIST Webbook
rinpol	2683.00	NIST Webbook
rinpol	2662.00	NIST Webbook
rinpol	2662.00	NIST Webbook
rinpol	2707.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C117895&Units=SI

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices