TRIFLUOMEPRAZINE

Other names: 10-[3-(Dimethylamino)-2-methylpropyl]-2-(trifluoromethyl)phenothiazine
Nortran [as maleate]
RP-7746
Inchi: InChI=1S/C19H21F3N2S/c1-13(11-23(2)3)12-24-15-6-4-5-7-17(15)25-18-9-8-14(10-16(1
InchiKey: ILBBYVOOXMPNTM-UHFFFAOYSA-N
Formula: C19H21F3N2S
SMILES: CC(CN(C)C)CN1c2ccccc2Sc2ccc(C(F)(F)F)cc21
Mol. weight [g/mol]: 366.45

Physical Properties

Property code	Value	Unit	Source
ie	7.29	eV	Cheméo Relay (1.0)
log10ws	-5.61		Cheméo Relay (1.0)
logp	5.506		Crippen Method
mcvol	261.810	ml/mol	McGowan Method
rinpol	2250.00		NIST Webbook
tf	413.45	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2622379&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tf:	Normal melting (fusion) point