

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]:	366.44
CAS:	2622-37-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.36		Crippen Method
logp	5.506		Crippen Method
mcvol	261.810	ml/mol	McGowan Method
rinpol	2250.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2622379&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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