Triflumizole

Other names:	1-(1-((4-Chloro-2-(trifluoromethyl)phenyl)imino)-2-propoxyethyl)-1H-imidazole 1H-Imidazole, 1-(1-((4-chloro-2-(trifluoromethyl)phenyl)imino)-2-propoxyethyl)- Benzenamine, 4-chloro-N-[1-(1H-imidazol-1-yl)-2-propoxyethylidene]-2-(trifluoromethyl)-, [N(E)]- N-[4-chloro-2-(trifluoromethyl)phenyl]-1-imidazol-1-yl-2-propoxyethanimine NF-114 Triflumizol Trifmine
Inchi:	InChI=1S/C15H15ClF3N3O/c1-2-7-23-9-14(22-6-5-20-10-22)21-13-4-3-11(16)8-12(13)15
InchiKey:	HSMVPDGQOIQYSR-UHFFFAOYSA-N
Formula:	C15H15ClF3N3O
SMILES:	CCCOCC(=Nc1ccc(Cl)cc1C(F)(F)F)n1ccnc1
Mol. weight [g/mol]:	345.75
CAS:	68694-11-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Aqueous Solubility Prediction Method
logp	4.560		Crippen Method
mcvol	228.050	ml/mol	McGowan Method
rinpol	2057.00		NIST Webbook
ripol	2981.00		NIST Webbook

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=C68694111&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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