RANITIDINE

Other names:	1,1-Ethenediamine, N-[2-[[[5-[(dimethylamino)methyl]-2-furanyl]methyl]thio]ethyl]-N'-methyl-2-nitro-
	N-(2-(((5-((dimethylamino)methyl)furan-2-yl)methyl)thio)ethyl)-N'-methyl-2-nitroethene-1,1
	N-[2-[[5-[(Dimethylamino)methyl]furfuryl]thio]ethyl]-N'-methyl-2-nitro-1,1-ethenediamine
	N-[2-[[5-[(Dimethylamino)methyl]furfuryl]thio]ethyl]-N'-methyl-2-nitro-1,1-ethylenediamine
Inchi:	InChI=1S/C13H22N4O3S/c1-14-13(9-17(18)19)15-6-7-21-10-12-5-4-11(20-12)8-16(2)3/h
InchiKey:	VMXUWOKSQNHOCA-UKTHLTGXSA-N
Formula:	C13H22N4O3S
SMILES:	CN/C(=C\[N+](=O)[O-])NCCSCc1ccc(CN(C)C)o1
Mol. weight [g/mol]:	314.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Aqueous Solubility Prediction Method
logp	1.459		Crippen Method
mcvol	239.850	ml/mol	McGowan Method
rinpol	2087.00		NIST Webbook
tf	406.15	K	Liquid pharmaceuticals formulation by eutectic formation

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Liquid pharmaceuticals formulation by eutectic formation:	https://www.doi.org/10.1016/j.fluid.2017.05.009
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66357355&Units=SI
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
tf:	Normal melting (fusion) point