N-(2-(((2-((dimethylamino)methyl)thiazol-4-yl)meth

Other names: N-{2-[({2-[(dimethylamino)methyl]-1,3-thiazol-4-yl}methyl)sulfanyl]ethyl}-N'-methyl-2-nitroe
nizatidine
Inchi: InChI=1S/C12H21N5O2S2/c1-13-11(6-17(18)19)14-4-5-20-8-10-9-21-12(15-10)7-16(2)3/
InchiKey: SGXXNSQHWDMGGP-UHFFFAOYSA-N
Formula: C12H21N5O2S2
SMILES: CNC(=C[N+](=O)[O-])NCCSCc1csc(CN(C)C)n1
Mol. weight [g/mol]: 331.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Cheméo Relay (1.0)
logp	1.323		Crippen Method
mcvol	246.220	ml/mol	McGowan Method
tf	401.62	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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):
Solubilities of Nizatidine in Water, Methanol, Ethanol, Acetone, and Ethyl Acetate from (273.15 to 343.15) K: https://www.doi.org/10.1021/je1000928

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point