

N-(2-(((2-((dimethylamino)methyl)thiazol-4-yl)methyl)sulfanyl)ethyl)-N'-methyl-2-nitroethanimide

Other names:	N-{2-[(2-[(dimethylamino)methyl]-1,3-thiazol-4-yl)methyl]sulfanyl}ethyl)-N'-methyl-2-nitroethanimide
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

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