

METHAZOLAMIDE

Other names:	2-Acetylimino-3-methyl-«delta»(4)-1,3,4-thiadiazoline-5-sulfonamide 5-Acetylimino-4-methyl-«delta»(2)-1,3,4-thiadiazoline-2-sulfonamide Acetamide, N-(4-methyl-2-sulfamoyl-«delta»2-1,3,4-thiadiazolin-5-ylidene)- Acetamide, N-[5-(aminosulfonyl)-3-methyl-1,3,4-thiadiazol-2(3H)-ylidene]- Methenamide N-(4-Methyl-2-sulfamoyl-«delta»2-1,3,4-thiadiazolin-5-ylidene)acetamide Naptazane Neptazane Neptazaneat
Inchi:	InChI=1S/C5H8N4O3S2/c1-3(10)7-4-9(2)8-5(13-4)14(6,11)12/h1-2H3,(H2,6,11,12)
InchiKey:	FLOSMHQXBMRNHR-UHFFFAOYSA-N
Formula:	C5H8N4O3S2
SMILES:	CC(=O)N=c1sc(S(N)(=O)=O)nn1C
Mol. weight [g/mol]:	236.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.87		Aqueous Solubility Prediction Method
logp	-1.424		Crippen Method
mcvol	147.780	ml/mol	McGowan Method
rinpol	2187.00		NIST Webbook
tf	486.65	K	Aqueous Solubility Prediction Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C554574&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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

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