Methazolamide

Other names: 2-Acetylimino-3-methyl-«delta»(4)-1,3,4-thiadiazoline-5-sulfonamide
2-Acetylimino-3-methyl-Â«deltaÂ»(4)-1,3,4-thiadiazoline-5-sulfonamide
5-Acetylimino-4-methyl-«delta»(2)-1,3,4-thiadiazoline-2-sulfonamide
5-Acetylimino-4-methyl-Â«deltaÂ»(2)-1,3,4-thiadiazoline-2-sulfonamide
Acetamide, N-(4-methyl-2-sulfamoyl-«delta»2-1,3,4-thiadiazolin-5-ylidene)-
Acetamide, N-(4-methyl-2-sulfamoyl-Â«deltaÂ»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
N-(4-Methyl-2-sulfamoyl-Â«deltaÂ»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]: 236.27

CAS: 554-57-4

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/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C554574&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
tf:	Normal melting (fusion) point