5-Acetamido-1,3,4-thiadiazole-2-sulfonamide

Other names:

1,3,4-Thiadiazole-2-sulfonamide, 5-acetamido-
2-Acetamido-1,3,4-thiadiazole-5-sulfonamide
2-Acetamido-5-sulfonamido-1,3,4-thiadiazole
2-Acetylamino-1,3,4-thiadiazole-5-sulfonamide
4-Diamox
5-Acetamide-1,3,4-thiadiazole-2-sulfonamide
5-Acetamido-1,3,4-thiadiazol-2-sulfonamide
Acetamide, N-(5-sulfamoyl-1,3,4-thiadiazol-2-yl)-
Acetamide, N-[5-(aminosulfonyl)-1,3,4-thiadiazol-2-yl]-
Acetamidothiadiazolesulfonamide
Acetamox
Acetazolamid
Acetazoleamide
Acetozalamide
Atenezol
Carbonic anhydrase inhibitor 6063
Carbonic anhydrase inhibitor no. 6063
Cidamex
Defiltran
Dehydratin
Diacarb
Diakarb
Diamox
Didoc
Diluran
Diuramid
Diureticum-holzinger
Diuriwas
Diutazol
Donmox
Duiramid
Edemox
Eumicton
Fonurit
Glaupax
Glupax
N-(5-(Aminosulfonyl)-1,3,4-thiadiazol-2-yl)acetamide
N-(5-Sulfamoyl-1,3,4-thiadiazol-2-yl)acetamide
NSC 145177
Natrionex

	Nephramid
	Nephramide
	Phonurit
	SK-acetazolamide
	Vetamox
	acetazolamide
Inchi:	InChI=1S/C4H6N4O3S2/c1-2(9)6-3-7-8-4(12-3)13(5,10)11/h1H3,(H2,5,10,11)(H,6,7,9)
InchiKey:	BZKPWHYZMXOIDC-UHFFFAOYSA-N
Formula:	C4H6N4O3S2
SMILES:	CC(=O)Nc1nnc(S(N)(=O)=O)s1
Mol. weight [g/mol]:	222.25
CAS:	59-66-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Aqueous Solubility Prediction Method
log10ws	-2.36		Estimated Solubility Method
log10ws	-2.49		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.856		Crippen Method
mcvol	133.690	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	28.60	kJ/mol	532.20	NIST Webbook

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume