

acetyl sulfisoxazole

Other names:

Acetamide, N-[(4-aminophenyl)sulfonyl]-N-(3,4-dimethyl-5-isoxazolyl)-
N-(3,4-Dimethyl-5-isoxazolyl)-N-sulfanilylacetamide
Lipo Gantrisin
Acetyl sulfisoxazole

Inchi:

InChI=1S/C13H15N3O4S/c1-8-9(2)15-20-13(8)16(10(3)17)21(18,19)12-6-4-11(14)5-7-12

InchiKey:

JFNWFXVFBDDWCX-UHFFFAOYSA-N

Formula:

C13H15N3O4S

SMILES:

CC(=O)N(c1onc(C)c1C)S(=O)(=O)c1ccc(N)cc1

Mol. weight [g/mol]:

309.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Aqueous Solubility Prediction Method
logp	1.615		Crippen Method
mcvol	216.280	ml/mol	McGowan Method
tf	466.65	K	Aqueous Solubility Prediction Method

Sources

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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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