

Sulfisoxazole Acetyl

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

Acetamide, N-(3,4-dimethyl-5-isoxazolyl)-N-sulfanilyl-
N-3,4-dimethylisoxazol-5-yl-N-sulphanilylacetamide

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]:

309.34

CAS:

80-74-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.15		Crippen Method
logp	1.615		Crippen Method
mcvol	216.280	ml/mol	McGowan Method

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C80740&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

Latest version available from:

<https://www.chemeo.com/cid/105-371-3/Sulfisoxazole-Acetyl.pdf>

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