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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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