

Acetamide, N-[4-[[[(5-methyl-3-isoxazolyl)amino]sulfonyl]phenyl]phenyl]acetamide

Other names:

N-[4-[[[(5-methylisoxazol-3-yl)amino]sulphonyl]phenyl]phenyl]acetamide

N4-Acetyl sulfamethoxazol

Inchi: InChI=1S/C12H13N3O4S/c1-8-7-12(14-19-8)15-20(17,18)11-5-3-10(4-6-11)13-9(2)16/h3

InchiKey: GXPIUNZCALHVBA-UHFFFAOYSA-N

Formula: C12H13N3O4S

SMILES: CC(O)=Nc1ccc(S(=O)(=O)Nc2cc(C)on2)cc1

Mol. weight [g/mol]: 295.31

CAS: 21312-10-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.34		Crippen Method
logp	2.392		Crippen Method
mcvol	202.190	ml/mol	McGowan Method
rinpol	2648.00		NIST Webbook
rinpol	2648.00		NIST Webbook

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=C21312107&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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