

Sulfamethazine, N-acetyl-

Other names:	N4-Acetyl sulfadimidin
Inchi:	InChI=1S/C14H16N4O3S/c1-9-8-10(2)16-14(15-9)18-22(20,21)13-6-4-12(5-7-13)17-11(3
InchiKey:	LJKAKWDUZRJNPJ-UHFFFAOYSA-N
Formula:	C14H16N4O3S
SMILES:	CC(=O)Nc1ccc(S(=O)(=O)Nc2nc(C)cc(C)n2)cc1
Mol. weight [g/mol]:	320.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Crippen Method
logp	1.853		Crippen Method
mcvol	230.180	ml/mol	McGowan Method
rinpol	2913.00		NIST Webbook
rinpol	2890.00		NIST Webbook
rinpol	2913.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U365474&Units=SI
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

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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