N4-Acetyl sulfadiazin

Inchi: InChI=1S/C12H12N4O3S/c1-9(17)15-10-3-5-11(6-4-10)20(18,19)16-12-13-7-2-8-14-12/h
InchiKey: NJIZUWGMNCUKGU-UHFFFAOYSA-N
Formula: C12H12N4O3S
SMILES: CC(=O)Nc1ccc(S(=O)(=O)Nc2ncccn2)cc1
Mol. weight [g/mol]: 292.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.71		Crippen Method
logp	1.236		Crippen Method
mcvol	202.000	ml/mol	McGowan Method
rinpol	2858.00		NIST Webbook

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=R525550&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
rinpol: Non-polar retention indices