N4-Acetyl sulfameter

Inchi: InChI=1S/C13H14N4O4S/c1-9(18)16-10-3-5-12(6-4-10)22(19,20)17-13-14-7-11(21-2)8-1
InchiKey: GUKOCAZFTOVPIS-UHFFFAOYSA-N
Formula: C13H14N4O4S
SMILES: COc1cnc(NS(=O)(=O)c2ccc(NC(C)=O)cc2)nc1
Mol. weight [g/mol]: 322.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	1.244		Crippen Method
mcvol	221.960	ml/mol	McGowan Method
rinpol	3090.00		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=R525585&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