

Dimetotiazine M (hydroxy-), acetylated

Inchi: InChI=1S/C21H27N3O4S2/c1-14(22(3)4)13-24-18-9-7-16(28-15(2)25)11-21(18)29-20-10
InchiKey: HGUXYQMMOBNHNY-UHFFFAOYSA-N
Formula: C21H27N3O4S2
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccc(S(=O)(=O)N(C)C)cc1N2CC(C)N(C)C
Mol. weight [g/mol]: 449.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.18		Crippen Method
logp	3.415		Crippen Method
mcvol	330.190	ml/mol	McGowan Method
rinpol	3200.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R314320&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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<https://www.chemeo.com/cid/61-107-5/Dimetotiazine-M-hydroxy-acetylated.pdf>

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