Dimetotiazine M (bis-nor-), acetylated

Inchi: InChI=1S/C19H23N3O3S2/c1-13(20-14(2)23)12-22-16-7-5-6-8-18(16)26-19-10-9-15(11-
InchiKey: SBEQDNNGJKDGFQ-UHFFFAOYSA-N
Formula: C19H23N3O3S2
SMILES: CC(=O)NC(C)CN1c2ccccc2Sc2ccc(S(=O)(=O)N(C)C)cc21
Mol. weight [g/mol]: 405.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	3.064		Crippen Method
mcvol	296.140	ml/mol	McGowan Method
rinpol	3380.00		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=R314315&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