

Thiethylperazine M (nor-), acetylated

Inchi: InChI=1S/C23H29N3OS2/c1-3-28-19-9-10-23-21(17-19)26(20-7-4-5-8-22(20)29-23)12-6
InchiKey: JHZPRQMSMGDQPD-UHFFFAOYSA-N
Formula: C23H29N3OS2
SMILES: CCSc1ccc2c(c1)N(CCCN1CCN(C(C)=O)CC1)c1cccc1S2
Mol. weight [g/mol]: 427.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	4.955		Crippen Method
mcvol	329.900	ml/mol	McGowan Method
rinpole	3650.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R314528&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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