

# Dimetotiazine M (nor-), acetylated

**Inchi:** InChI=1S/C20H25N3O3S2/c1-14(22(5)15(2)24)13-23-17-8-6-7-9-19(17)27-20-11-10-16(21)  
**InchiKey:** RKSUYMQRUONBBE-UHFFFAOYSA-N  
**Formula:** C20H25N3O3S2  
**SMILES:** CC(=O)N(C)C(C)CN1c2ccccc2Sc2ccc(S(=O)(=O)N(C)C)cc21  
**Mol. weight [g/mol]:** 419.56

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.06		Crippen Method
logp	3.406		Crippen Method
mcvol	310.230	ml/mol	McGowan Method
rinpol	3360.00		NIST Webbook
rinpol	3360.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R314335&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

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