

Mequitazine M (sulfone)

Inchi: InChI=1S/C20H22N2O2S/c23-25(24)19-7-3-1-5-17(19)22(18-6-2-4-8-20(18)25)14-16-13
InchiKey: XPKWOPYSZJPRLJ-UHFFFAOYSA-N
Formula: C20H22N2O2S
SMILES: O=S1(=O)c2ccccc2N(CC2CN3CCC2CC3)c2ccccc21
Mol. weight [g/mol]: 354.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	3.313		Crippen Method
mcvol	260.610	ml/mol	McGowan Method
rinpol	3250.00		NIST Webbook
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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=R314439&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/50-945-7/Mequitazine-M-sulfone.pdf>

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