

Thioridazine M (oxo-)

Inchi: InChI=1S/C21H24N2OS2/c1-22-15(6-5-9-21(22)24)12-13-23-17-7-3-4-8-19(17)26-20-11
InchiKey: ZNUYBUSUMRYHBP-UHFFFAOYSA-N
Formula: C21H24N2OS2
SMILES: CSc1ccc2c(c1)N(CCC1CCCC(=O)N1C)c1ccccc1S2
Mol. weight [g/mol]: 384.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.86		Crippen Method
logp	5.412		Crippen Method
mcvol	291.740	ml/mol	McGowan Method
rinpola	3500.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R212858&Units=SI>
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>

Legend

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

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<https://www.chemeo.com/cid/84-702-9/Thioridazine-M-oxo.pdf>

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