

2-Dimethylamino-1-phenothiazin-10-yl-propan-1-one

(from Secergan)
InChI: InChI=1S/C17H18N2OS/c1-4-17(20)19-13-7-5-6-8-15(13)21-16-11-12(18(2)3)9-10-14(16)
InChIKey: XFNLEWZVQWHDAA-UHFFFAOYSA-N

Formula: C17H18N2OS
SMILES: CCC(=O)N1c2ccccc2Sc2cc(N(C)C)ccc21
Mol. weight [g/mol]: 298.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.36		Crippen Method
logp	4.292		Crippen Method
mcvol	229.890	ml/mol	McGowan Method
rinpol	2310.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R489182&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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
rinpol: Non-polar retention indices

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