2-Dimethylamino-1-phenothiazin-10-yl-propan-1-o (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: XPNLEWZVQWHDAA-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/ci990307l
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
rinpol: Non-polar retention indices