

Levomepromazine M (HO-), monoacetylated

Inchi: InChI=1S/C21H26N2O3S/c1-14(12-22(3)4)13-23-16-8-6-7-9-20(16)27-21-11-19(26-15(2
InchiKey: UUONPBYOPXKDSU-AWEZLNQCLSA-N
Formula: C21H26N2O3S
SMILES: COc1cc2c(cc1OC(C)=O)Sc1ccccc1N2CC(C)CN(C)C
Mol. weight [g/mol]: 386.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.69		Crippen Method
logp	4.421		Crippen Method
mcvol	297.990	ml/mol	McGowan Method
rinpola	2747.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R310388&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

Latest version available from:

<https://www.chemeo.com/cid/17-400-8/Levomepromazine-M-HO-monoacetylated.pdf>

Generated by Cheméo on 2024-04-19 14:27:54.140766209 +0000 UTC m=+15826123.061343521.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.