

10H-Phenothiazin-3-ol, 10-[3-(dimethylamino)propyl]-, acetate (ester)

Other names: Promazine M (HO-), monoacetylated
Inchi: InChI=1S/C19H22N2O2S/c1-14(22)23-15-9-10-17-19(13-15)24-18-8-5-4-7-16(18)21(17)
InchiKey: WZQPRXUQVBEBTL-UHFFFAOYSA-N
Formula: C19H22N2O2S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1cccc1N2CCCN(C)C
Mol. weight [g/mol]: 342.45
CAS: 56438-23-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.40		Crippen Method
logp	4.166		Crippen Method
mcvol	263.940	ml/mol	McGowan Method
rinpol	2709.00		NIST Webbook
rinpol	2781.00		NIST Webbook
rinpol	2709.00		NIST Webbook

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=C56438234&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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