

Acepromethazine

Other names: Aceprometazine
Inchi: InChI=1S/C19H22N2OS/c1-13(20(3)4)12-21-16-7-5-6-8-18(16)23-19-10-9-15(14(2)22)1
InchiKey: XLOQNFNTQIRSOX-UHFFFAOYSA-N
Formula: C19H22N2OS
SMILES: CC(=O)c1ccc2c(c1)N(CC(C)N(C)C)c1ccccc1S2
Mol. weight [g/mol]: 326.46
CAS: 13461-01-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	4.442		Crippen Method
mcvol	258.070	ml/mol	McGowan Method
rmpol	2626.00		NIST Webbook
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Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13461013&Units=SI>

Legend

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

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