

8-Methoxyloxapine

Inchi: InChI=1S/C19H20ClN3O2/c1-22-8-10-23(11-9-22)19-14-12-13(20)6-7-15(14)25-17-5-3-4
InchiKey: VSQGILJVCFFROT-UHFFFAOYSA-N
Formula: C19H20ClN3O2
SMILES: COc1cccc2c1N=C(N1CCN(C)CC1)c1cc(Cl)ccc1O2
Mol. weight [g/mol]: 357.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	3.780		Crippen Method
mcvol	258.950	ml/mol	McGowan Method
rinpol	2810.00		NIST Webbook
rinpol	2810.00		NIST Webbook

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=R21827&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/99-911-1/8-Methoxyloxapine.pdf>

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