

Olanzapine AC

Inchi: InChI=1S/C19H22N4OS/c1-13-12-15-18(22-10-8-21(3)9-11-22)20-16-6-4-5-7-17(16)23(14)24
InchiKey: ACCNIDYFTWFBGF-UHFFFAOYSA-N
Formula: C19H22N4OS
SMILES: CC(=O)N1c2ccccc2N=C(N2CCN(C)CC2)c2cc(C)sc21
Mol. weight [g/mol]: 354.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	3.380		Crippen Method
mcvol	267.170	ml/mol	McGowan Method
rinpola	2780.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R331152&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.cheméo.com/cid/31-372-4/Olanzapine-AC.pdf>

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