

Olanzapine-M (nor-) 2AC

Inchi: InChI=1S/C20H22N4O2S/c1-13-12-16-19(23-10-8-22(9-11-23)14(2)25)21-17-6-4-5-7-18
InchiKey: SWZDOVRVQPEIBC-UHFFFAOYSA-N
Formula: C20H22N4O2S
SMILES: CC(=O)N1CCN(C2=Nc3ccccc3N(C(C)=O)c3sc(C)cc32)CC1
Mol. weight [g/mol]: 382.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	3.297		Crippen Method
mcvol	282.830	ml/mol	McGowan Method
rinpola	3200.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R331167&Units=SI>

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/12-523-7/Olanzapine-M-nor-2AC.pdf>

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