

Mirtazapine-M (oxo-)

Inchi: InChI=1S/C17H17N3O/c1-19-9-10-20-15(11-19)12-5-2-3-6-13(12)16(21)14-7-4-8-18-17(21)
InchiKey: RZDFSDWHGNDESU-UHFFFAOYSA-N
Formula: C17H17N3O
SMILES: CN1CCN2c3ncccc3C(=O)c3ccccc3C2C1
Mol. weight [g/mol]: 279.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	2.119		Crippen Method
mcvol	212.660	ml/mol	McGowan Method
rinpola	2655.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R331098&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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

Latest version available from:

<https://www.chemeo.com/cid/61-295-7/Mirtazapine-M-oxo.pdf>

Generated by Cheméo on 2024-04-18 00:08:29.410034558 +0000 UTC m=+15688158.330611881.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.