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(
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
rinpol	2655.00		NIST Webbook

Sources

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=R331098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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