

Oxatomide M (N-desalkyl), acetylated

Other names:	Norcyclizine, acetylated
Inchi:	InChI=1S/C19H22N2O/c1-16(22)20-12-14-21(15-13-20)19(17-8-4-2-5-9-17)18-10-6-3-7-
InchiKey:	XFKXNYYYOGBBGS-UHFFFAOYSA-N
Formula:	C19H22N2O
SMILES:	CC(=O)N1CCN(C(c2cccc2)c2cccc2)CC1
Mol. weight [g/mol]:	294.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Cheméo Relay (1.0)
logp	2.940		Crippen Method
mcvol	241.720	ml/mol	McGowan Method
rinpol	2525.00		NIST Webbook
rinpol	2525.00		NIST Webbook
rinpol	2525.00		NIST Webbook
tf	367.30	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R536228&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

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