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(c2ccccc2)c2ccccc2)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/ci990307l
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