

Buclizine M (N-desalkyl), acetylated

Inchi: InChI=1S/C19H21ClN2O/c1-15(23)21-11-13-22(14-12-21)19(16-5-3-2-4-6-16)17-7-9-18(20)
InchiKey: SQGNETKFPNXNSE-UHFFFAOYSA-N
Formula: C19H21ClN2O
SMILES: CC(=O)N1CCN(C(c2ccccc2)c2ccc(Cl)cc2)CC1
Mol. weight [g/mol]: 328.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	3.594		Crippen Method
mcvol	253.960	ml/mol	McGowan Method
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R536124&Units=SI>
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>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/14-657-7/Buclizine-M-N-desalkyl-acetylated.pdf>

Generated by Cheméo on 2024-04-25 19:47:31.142718939 +0000 UTC m=+16363700.063296251.

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