

Buclizine M (carbinol), acetylated

Inchi: InChI=1S/C30H35ClN2O2/c1-23(34)35-30(26-8-6-5-7-9-26,27-14-16-28(31)17-15-27)33
InchiKey: NQQNLEXZNDYJOJ-UHFFFAOYSA-N
Formula: C30H35ClN2O2
SMILES: CC(=O)OC(c1ccccc1)(c1ccc(Cl)cc1)N1CCN(Cc2ccc(C(C)(C)C)cc2)CC1
Mol. weight [g/mol]: 491.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.17		Crippen Method
logp	6.220		Crippen Method
mcvol	391.060	ml/mol	McGowan Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R536080&Units=SI>

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/121-018-7/Buclizine-M-carbinol-acetylated.pdf>

Generated by Cheméo on 2024-04-29 05:06:56.903623892 +0000 UTC m=+16656465.824201204.

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