

Medazepam M (nor-), acetylated

Inchi: InChI=1S/C17H15ClN2O/c1-12(21)20-10-9-19-17(13-5-3-2-4-6-13)15-11-14(18)7-8-16(1)
InchiKey: OARDNFYVAOWKLN-UHFFFAOYSA-N
Formula: C17H15ClN2O
SMILES: CC(=O)N1CCN=C(c2ccccc2)c2cc(Cl)ccc21
Mol. weight [g/mol]: 298.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	3.544		Crippen Method
mcvol	221.480	ml/mol	McGowan Method
rinpola	2470.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R313278&Units=SI>

Legend

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

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