LORCAINIDE, M(DESACYL-), AC

Inchi: InChI=1S/C16H23ClN2O/c1-12(2)18-10-8-16(9-11-18)19(13(3)20)15-6-4-14(17)5-7-15/h
InchiKey: KZATYWDDOUULEZ-UHFFFAOYSA-N
Formula: C16H23ClN2O
SMILES: CC(=O)N(c1ccc(Cl)cc1)C1CCN(C(C)C)CC1
Mol. weight [g/mol]: 294.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	3.566		Crippen Method
mcvol	235.450	ml/mol	McGowan Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R255177&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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