

Nimodipine M (dehydro-desisopropyl-O-desmethyl, methyl ester)

InChI: InChI=1S/C19H20N2O7/c1-11-15(18(22)27-4)17(13-6-5-7-14(10-13)21(24)25)16(12(2)20)26
InChIKey: OKYRJOYGNPZZCD-UHFFFAOYSA-N
Formula: C19H20N2O7
SMILES: COCCOC(=O)c1c(C)nc(C)c(C(=O)OC)c1-c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 388.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.85		Crippen Method
logp	2.863		Crippen Method
mcvol	279.200	ml/mol	McGowan Method
rinpol	2665.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R89730&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/15-802-4/Nimodipine-M-dehydro-desisopropyl-O-desmethyl-methyl-ester.pdf>

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