Nitrendipine M (dehydro-desethyl, methyl ester)

Other names: Nimodipine M (dehydro-desisopropyl-desmethoxyethyl, methyl ester)
Nicardipine M (dehydro-desbenzylmethylaminoethyl, methyl ester)

Inchi: InChI=1S/C17H16N2O6/c1-9-13(16(20)24-3)15(14(10(2)18-9)17(21)25-4)11-6-5-7-12(8-

InchiKey: WLSSRGYMMSQMGL-UHFFFAOYSA-N

Formula: C17H16N2O6

SMILES: COC(=O)c1c(C)nc(C)c(C(=O)OC)c1-c1cccc([N+](=O)[O-])c1

Mol. weight [g/mol]: 344.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.93		Crippen Method
logp	2.847		Crippen Method
mcvol	245.150	ml/mol	McGowan Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R89655&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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