Nifedipine M (dehydro)

Inchi: InChI=1S/C17H16N2O6/c1-9-13(16(20)24-3)15(14(10(2)18-9)17(21)25-4)11-7-5-6-8-12(
InchiKey: UMQHJQGNGLQJPF-UHFFFAOYSA-N
Formula: C17H16N2O6
SMILES: COC(=O)c1c(C)nc(C)c(C(=O)OC)c1-c1ccccc1[N+](=O)[O-]
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	2255.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R89669&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