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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R89669&Units=SI

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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