Nilvadipine M (dehydro)

Inchi: InChI=1S/C19H17N3O6/c1-10(2)28-19(24)17-14(9-20)21-11(3)15(18(23)27-4)16(17)12-6
InchiKey: ISSSWUSFUCIVHT-UHFFFAOYSA-N
Formula: C19H17N3O6
SMILES: COC(=O)c1c(C)nc(C#N)c(C(=O)OC(C)C)c1-c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 383.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.75		Crippen Method
logp	3.189		Crippen Method
mcvol	274.710	ml/mol	McGowan Method
rinpol	2565.00		NIST Webbook
rinpol	2565.00		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=R89687&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.