Nifedipine M (dehydro-bis-carboxy, methyl ester)

Inchi: InChI=1S/C18H16N2O8/c1-9-12(16(21)26-2)13(10-7-5-6-8-11(10)20(24)25)14(17(22)27-

InchiKey: RVORVWKPTSHPSE-UHFFFAOYSA-N

Formula: C18H16N2O8

SMILES: COC(=O)c1nc(C)c(C(=O)OC)c(-c2ccccc2[N+](=O)[O-])c1C(=O)OC

Mol. weight [g/mol]: 388.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	2.325		Crippen Method
mcvol	266.680	ml/mol	McGowan Method
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R89673&Units=SI

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

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.