

Nitrendipine M (dehydro)

Inchi: InChI=1S/C18H18N2O6/c1-5-26-18(22)15-11(3)19-10(2)14(17(21)25-4)16(15)12-7-6-8-1
InchiKey: YEHVABIPGJLMET-UHFFFAOYSA-N
Formula: C18H18N2O6
SMILES: CCOC(=O)c1c(C)nc(C)c(C(=O)OC)c1-c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 358.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.35		Crippen Method
logp	3.237		Crippen Method
mcvol	259.240	ml/mol	McGowan Method
rinpol	2370.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R89801&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

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<https://www.chemeo.com/cid/114-831-2/Nitrendipine-M-dehydro.pdf>

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