

Nicardipine M (dehydro-desamino-hydroxy)

Inchi: InChI=1S/C18H18N2O7/c1-10-14(17(22)26-3)16(12-5-4-6-13(9-12)20(24)25)15(11(2)19-
InchiKey: DCIMTQCMPVHZFX-UHFFFAOYSA-N
Formula: C18H18N2O7
SMILES: COC(=O)c1c(C)nc(C)c(C(=O)OCCO)c1-c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 374.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.61		Crippen Method
logp	2.209		Crippen Method
mcvol	265.110	ml/mol	McGowan Method
rinpola	2665.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R89641&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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