

Nilvadipine M (dehydro-desisopropyl, methyl ester)

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|----------------------|--|
| Inchi: | InChI=1S/C17H13N3O6/c1-9-13(16(21)25-2)14(10-5-4-6-11(7-10)20(23)24)15(17(22)26- |
| InchiKey: | NNHXMCIQQSAQLS-UHFFFAOYSA-N |
| Formula: | C17H13N3O6 |
| SMILES: | COC(=O)c1c(C)nc(C#N)c(C(=O)OC)c1-c1cccc([N+](=O)[O-])c1 |
| Mol. weight [g/mol]: | 355.30 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.80 | | Crippen Method |
| logp | 2.410 | | Crippen Method |
| mcvol | 246.530 | ml/mol | McGowan Method |
| rinpol | 2520.00 | | NIST Webbook |
| rinpol | 2520.00 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| 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=R89691&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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/117-705-9/Nilvadipine-M-dehydro-desisopropyl-methyl-ester.pdf>

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