

Nimodipine M (dehydro-O-desmethyl-carboxy, methyl ester)

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|-----------------------------|---|
| Inchi: | InChI=1S/C20H20N2O8/c1-11(2)30-20(25)17-12(3)21-9-15(19(24)29-10-16(23)28-4)18(|
| InchiKey: | OUNDLGCXBQDMKZ-UHFFFAOYSA-N |
| Formula: | C20H20N2O8 |
| SMILES: | COC(=O)COC(=O)c1cnc(C)c(C(=O)OC(C)C)c1-c1cccc([N+](=O)[O-])c1 |
| Mol. weight [g/mol]: | 416.38 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.10 | | Crippen Method |
| logp | 2.860 | | Crippen Method |
| mcvol | 294.860 | ml/mol | McGowan Method |
| rinpola | 2740.00 | | NIST Webbook |
| rinpola | 2740.00 | | NIST Webbook |

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=R328473&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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<https://www.cheméo.com/cid/62-570-0/Nimodipine-M-dehydro-O-desmethyl-carboxy-methyl-ester.pdf>

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