

Felodipine M (dehydro-desethyl, methyl ester)

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|-----------------------------|--|
| Inchi: | InChI=1S/C17H15Cl2NO4/c1-8-12(16(21)23-3)14(10-6-5-7-11(18)15(10)19)13(9(2)20-8) |
| InchiKey: | GJWDEVJSJBHKJAL-UHFFFAOYSA-N |
| Formula: | C17H15Cl2NO4 |
| SMILES: | <chem>COC(=O)c1c(C)nc(C)c(C(=O)OC)c1-c1cccc(Cl)c1Cl</chem> |
| Mol. weight [g/mol]: | 368.21 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.65 | | Crippen Method |
| logp | 4.245 | | Crippen Method |
| mcvol | 252.210 | ml/mol | McGowan Method |
| rinpol | 2235.00 | | NIST Webbook |
| rinpol | 2235.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R89605&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/117-138-9/Felodipine-M-dehydro-desethyl-methyl-ester.pdf>

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