# Dimethylphenobarbital

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|---|---|
| **Other names:** | 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-1,3-dimethyl-5-phenyl-<br>Barbituric acid, 5-ethyl-1,3-dimethyl-5-phenyl-<br>N,N'-Dimethylphenobarbital<br>1,3-Dimethylphenobarbital<br>1,3-Dimethylphenobarbitone<br>Barbituric acid, 1,3-dimethyl-5-ethyl-5-phenyl-<br>1,3-Dimethyl-5-ethyl-5-phenylbarbituric acid<br>2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,3-dimethyl-5-ethyl-5-phenyl-<br>5-Ethyl-1,3-dimethyl-5-phenylbarbituric acid<br>1,3-Dimethyl derivative of Phenobarbitol<br>Phenobarbitone-permethylated<br>Methylphenobarbitone-permethylated<br>N,N-Dimethyl-5-ethyl-5-phenylbarbituric acid<br>Phenobarbital di-methyl derivative<br>Mephobarbital Me<br>Mephobarbital permethylated<br>Phenobarbital, 1,3-dimethyl<br>Phenobarbital, permethyl<br>Phenobarbital permethylated<br>Methylphenobarbital, permethylated<br>Phenobarbital Me |
| **Inchi:** | InChI=1S/C14H16N2O3/c1-4-14(10-8-6-5-7-9-10)11(17)15(2)13(19)16(3)12(14)18/h5-9H |
| **InchiKey:** | RPJARFKGODFVHL-UHFFFAOYSA-N |
| **Formula:** | C14H16N2O3 |
| **SMILES:** | CCC1(c2ccccc2)C(=O)N(C)C(=O)N(C)C1=O |
| **Mol. weight [g/mol]:** | 260.29 |
| **CAS:** | 730-66-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -1.80 | | Crippen Method |
| logp | 1.385 | | Crippen Method |
| mcvol | 198.170 | ml/mol | McGowan Method |
| rinpol | 1880.00 | | NIST Webbook |
| rinpol | 1880.00 | | NIST Webbook |
| rinpol | 1881.00 | | NIST Webbook |

| | | |
|---|---|---|
| rinpol | 1832.00 | NIST Webbook |
| rinpol | 1870.00 | NIST Webbook |
| rinpol | 1826.00 | NIST Webbook |
| rinpol | 1825.00 | NIST Webbook |
| rinpol | 1881.00 | NIST Webbook |
| rinpol | 1832.00 | NIST Webbook |
| rinpol | 1881.00 | NIST Webbook |
| rinpol | 1831.00 | NIST Webbook |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C730665&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices