

2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,5-diethyl-3-methyl-5-phenyl-

Other names:

N-Ethylmethobarbital

Mephobarbital perethylated

Inchi:

InChI=1S/C15H18N2O3/c1-4-15(11-9-7-6-8-10-11)12(18)16(3)14(20)17(5-2)13(15)19/h6

InchiKey:

MKNZJVPKBDCKQB-UHFFFAOYSA-N

Formula:

C15H18N2O3

SMILES:

CCN1C(=O)N(C)C(=O)C(CC)(c2ccccc2)C1=O

Mol. weight [g/mol]:

274.31

CAS:

55255-46-4

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.22 | | Crippen Method |
| logp | 1.775 | | Crippen Method |
| mcvol | 212.260 | ml/mol | McGowan Method |
| rinpol | 1904.00 | | NIST Webbook |
| rinpol | 1904.00 | | NIST Webbook |

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C55255464&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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 |

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