

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-cyclohepten-1-yl)-5-ethyl-1,3-dimethyl-

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|-----------------------------|--|
| Other names: | Heptabarbitone-permethylated Heptabarbital, 1,3-dimethyl Heptabarbital permethylated |
| Inchi: | InChI=1S/C15H22N2O3/c1-4-15(11-9-7-5-6-8-10-11)12(18)16(2)14(20)17(3)13(15)19/h9 |
| InchiKey: | IOWZYALHIKMITA-UHFFFAOYSA-N |
| Formula: | C15H22N2O3 |
| SMILES: | CCC1(C2=CCCCC2)C(=O)N(C)C(=O)N(C)C1=O |
| Mol. weight [g/mol]: | 278.35 |
| CAS: | 54965-32-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.95 | | Crippen Method |
| logp | 2.324 | | Crippen Method |
| mcvol | 220.860 | ml/mol | McGowan Method |
| rinpol | 1988.00 | | NIST Webbook |
| rinpol | 1988.00 | | 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=C54965321&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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