

Barbituric acid, 5-allyl-5-(2-hydroxypropyl) permethylated

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C12H18N2O4/c1-5-6-12(7-8(2)15)9(16)13(3)11(18)14(4)10(12)17/h5,8,15H,1,6 |
| InchiKey: | OTFYIZHYJNTWHY-UHFFFAOYSA-N |
| Formula: | C12H18N2O4 |
| SMILES: | C=CCC1(CC(C)O)C(=O)N(C)C(=O)N(C)C1=O |
| Mol. weight [g/mol]: | 254.28 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.17 | | Crippen Method |
| logp | 0.370 | | Crippen Method |
| mcvol | 195.320 | ml/mol | McGowan Method |
| rinpol | 1670.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R387754&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| 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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