# Aprobarbital

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|---|---|
| **Other names:** | 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylethyl)-5-(2-propenyl)- |
| | 5-Allyl-5-isopropyl-2,4,6(1H,3H,5H)-pyrimidinetrione |
| | 5-Allyl-5-isopropylbarbital |
| | 5-Allyl-5-isopropylbarbiturate |
| | 5-Allyl-5-isopropylbarbituric acid |
| | 5-Isopropyl-5-allylbarbituric acid |
| | 5-propan-2-yl-5-prop-2-enyl-1,3-diazinane-2,4,6-trione |
| | Allional |
| | Allonal |
| | Allylisopropylbarbituric acid |
| | Allylisopropylmalonylurea |
| | Allylpropymal |
| | Allypropymal |
| | Alurate |
| | Alurate Elixir Verdum |
| | Aprobarbita |
| | Aprobarbitone |
| | Aprozal |
| | Barbituric acid, 5-allyl-5-isopropyl- |
| | Isonal |
| | Isopropylallylbarbituric acid |
| | NSC 120769 |
| | Numal |
| | Propallylonal M (des-Br) |
| **Inchi:** | InChI=1S/C10H14N2O3/c1-4-5-10(6(2)3)7(13)11-9(15)12-8(10)14/h4,6H,1,5H2,2-3H3,(H |
| **InchiKey:** | UORJNBVJVRLXMQ-UHFFFAOYSA-N |
| **Formula:** | C10H14N2O3 |
| **SMILES:** | C=CCC1(C(C)C)C(=O)NC(=O)NC1=O |
| **Mol. weight [g/mol]:** | 210.23 |
| **CAS:** | 77-02-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -54.67 | kJ/mol | Joback Method |
| hf | -397.50 | kJ/mol | Joback Method |
| hfus | 20.10 | kJ/mol | Joback Method |

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|---|---|---|---|
| hvap | 62.33 | kJ/mol | Joback Method |
| log10ws | -1.71 | | Aqueous Solubility Prediction Method |
| log10ws | -1.71 | | Estimated Solubility Method |
| log10ws | -1.71 | | Aqueous and cosolvent solubility data for drug-like organic compounds |
| logp | 0.571 | | Crippen Method |
| mcvol | 161.270 | ml/mol | McGowan Method |
| pc | 3368.44 | kPa | Joback Method |
| rinpol | 1600.00 | | NIST Webbook |
| rinpol | 1594.00 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |
| rinpol | 1619.00 | | NIST Webbook |
| rinpol | 1610.00 | | NIST Webbook |
| rinpol | 1621.00 | | NIST Webbook |
| rinpol | 1594.00 | | NIST Webbook |
| rinpol | 1627.00 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |
| rinpol | 1627.00 | | NIST Webbook |
| rinpol | 1610.00 | | NIST Webbook |
| rinpol | 1592.00 | | NIST Webbook |
| rinpol | 1598.00 | | NIST Webbook |
| rinpol | 1610.00 | | NIST Webbook |
| rinpol | 1610.00 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |
| rinpol | 1617.00 | | NIST Webbook |
| rinpol | 1622.00 | | NIST Webbook |
| tb | 744.79 | K | Joback Method |
| tc | 1008.19 | K | Joback Method |
| tf | 414.72 | K | Aqueous Solubility Prediction Method |
| vc | 0.597 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 470.14 | J/mol×K | 744.79 | Joback Method |
| cpg | 487.71 | J/mol×K | 788.69 | Joback Method |
| cpg | 504.35 | J/mol×K | 832.59 | Joback Method |
| cpg | 520.07 | J/mol×K | 876.49 | Joback Method |
| cpg | 534.89 | J/mol×K | 920.39 | Joback Method |

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|---|---|---|---|---|
| cpg | 548.82 | J/mol×K | 964.29 | Joback Method |
| cpg | 561.87 | J/mol×K | 1008.19 | Joback Method |

# Sources

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|---|---|
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **Aqueous and cosolvent solubility data for drug-like organic compounds:** | https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/ |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C77021&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |