# 5-Ethyl-5-pentylbarbituric acid

**Inchi:** InChI=1S/C11H18N2O3/c1-3-5-6-7-11(4-2)8(14)12-10(16)13-9(11)15/h3-7H2,1-2H3,(H2
**InchiKey:** XYGXSCVUMIDZRR-UHFFFAOYSA-N
**Formula:** C11H18N2O3
**SMILES:** CCCCCC1(CC)C(=O)NC(=O)NC1=O
**Mol. weight [g/mol]:** 226.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -131.65 | kJ/mol | Joback Method |
| hf | -538.29 | kJ/mol | Joback Method |
| hfus | 27.49 | kJ/mol | Joback Method |
| hvap | 65.61 | kJ/mol | Joback Method |
| log10ws | -2.34 | | Aqueous and cosolvent solubility data for drug-like organic compounds |
| logp | 1.329 | | Crippen Method |
| mcvol | 179.660 | ml/mol | McGowan Method |
| pc | 2862.74 | kPa | Joback Method |
| tb | 771.43 | K | Joback Method |
| tc | 1018.96 | K | Joback Method |
| tf | 659.73 | K | Joback Method |
| vc | 0.677 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 549.70 | J/mol×K | 771.43 | Joback Method |
| cpg | 567.97 | J/mol×K | 812.69 | Joback Method |
| cpg | 585.29 | J/mol×K | 853.94 | Joback Method |
| cpg | 601.66 | J/mol×K | 895.20 | Joback Method |
| cpg | 617.09 | J/mol×K | 936.45 | Joback Method |
| cpg | 631.61 | J/mol×K | 977.71 | Joback Method |
| cpg | 645.20 | J/mol×K | 1018.96 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

| | |
|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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