

# 5-Ethyl-5-pentylbarbituric acid

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | 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 |
| <b>InchiKey:</b>            | XYGXSCVUMIDZRR-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C11H18N2O3  |
| <b>SMILES:</b>              | CCCCC1(CC)C(=O)NC(=O)NC1=O  |
| <b>Mol. weight [g/mol]:</b> | 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   | m <sup>3</sup> /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

|   |   |
|---|---|
| <b>Joback Method:</b>   | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                     |
| <b>Aqueous and cosolvent solubility data for drug-like organic compounds:</b> | <a href="https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/">https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/</a> |
| <b>McGowan Method:</b>  | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>     |
| <b>Crippen Method:</b>  | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                 |

# Legend

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

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