

# Pentylone

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C13H17NO3/c1-3-4-10(14-2)13(15)9-5-6-11-12(7-9)17-8-16-11/h5-7,10,14H,3 |
| <b>InchiKey:</b>            | DFMLULIEUXXSA-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C13H17NO3  |
| <b>SMILES:</b>              | CCCC(NC)C(=O)c1ccc2c(c1)OCO2   |
| <b>Mol. weight [g/mol]:</b> | 235.28   |
| <b>CAS:</b>                 | 698963-77-8  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 5.98    | kJ/mol               | Joback Method  |
| hf            | -333.31 | kJ/mol               | Joback Method  |
| hfus          | 38.89   | kJ/mol               | Joback Method  |
| hvap          | 70.17   | kJ/mol               | Joback Method  |
| log10ws       | -3.32   |                      | Crippen Method |
| logp          | 1.986   |                      | Crippen Method |
| mcvol         | 182.700 | ml/mol               | McGowan Method |
| pc            | 2668.02 | kPa                  | Joback Method  |
| rinpol        | 1887.80 |                      | NIST Webbook   |
| rinpol        | 1887.80 |                      | NIST Webbook   |
| tb            | 702.39  | K                    | Joback Method  |
| tc            | 922.56  | K                    | Joback Method  |
| tf            | 450.64  | K                    | Joback Method  |
| vc            | 0.691   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 513.03 | J/mol×K | 702.39          | Joback Method |
| cpg           | 527.11 | J/mol×K | 739.09          | Joback Method |
| cpg           | 540.25 | J/mol×K | 775.78          | Joback Method |
| cpg           | 552.50 | J/mol×K | 812.48          | Joback Method |
| cpg           | 563.95 | J/mol×K | 849.17          | Joback Method |
| cpg           | 574.66 | J/mol×K | 885.87          | Joback Method |
| cpg           | 584.69 | J/mol×K | 922.56          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                           |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C698963778&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C698963778&amp;Units=SI</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>                                       |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                               |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>r in pol:</b> | Non-polar retention indices                     |
| <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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