

# cis-DL-Pinonic acid

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C10H16O3/c1-6(11)8-4-7(5-9(12)13)10(8,2)3/h7-8H,4-5H2,1-3H3,(H,12,13)/t7- |
| <b>InchiKey:</b>            | SIZDUQQDBXJXLQ-SFYZADRCSA-N  |
| <b>Formula:</b>             | C10H16O3   |
| <b>SMILES:</b>              | CC(=O)C1CC(CC(=O)O)C1(C)C  |
| <b>Mol. weight [g/mol]:</b> | 184.23   |
| <b>CAS:</b>                 | 17879-35-5   |

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| chs           | -5476.00 | kJ/mol  | NIST Webbook   |
| gf            | -333.60  | kJ/mol  | Joback Method  |
| hf            | -585.92  | kJ/mol  | Joback Method  |
| hfs           | -748.50  | kJ/mol  | NIST Webbook   |
| hfus          | 20.82    | kJ/mol  | Joback Method  |
| hvap          | 66.34    | kJ/mol  | Joback Method  |
| log10ws       | -1.56    |         | Crippen Method |
| logp          | 1.712    |         | Crippen Method |
| mcvol         | 149.910  | ml/mol  | McGowan Method |
| pc            | 2999.15  | kPa     | Joback Method  |
| tb            | 630.03   | K       | Joback Method  |
| tc            | 826.05   | K       | Joback Method  |
| tf            | 392.98   | K       | Joback Method  |
| vc            | 0.572    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 409.51 | J/molxK | 630.03          | Joback Method |
| cpg           | 422.36 | J/molxK | 662.70          | Joback Method |
| cpg           | 434.58 | J/molxK | 695.37          | Joback Method |
| cpg           | 446.27 | J/molxK | 728.04          | Joback Method |
| cpg           | 457.50 | J/molxK | 760.71          | Joback Method |
| cpg           | 468.37 | J/molxK | 793.38          | Joback Method |
| cpg           | 478.95 | J/molxK | 826.05          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>   |
| <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=C17879355&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17879355&amp;Units=SI</a> |

# Legend

|                 |  |
|-----------------|--|
| <b>chs:</b>     | Standard solid enthalpy of combustion                    |
| <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>hfs:</b>     | Solid phase 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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