

# Cyclopentane-1-carboxylic acid, 1-ethyl, methyl ester

|                      |                                                          |
|----------------------|----------------------------------------------------------|
| Other names:         | Cyclopentanecarboxylic acid, 1-ethyl, methyl ester       |
| Inchi:               | InChI=1S/C9H16O2/c1-3-9(8(10)11-2)6-4-5-7-9/h3-7H2,1-2H3 |
| InchiKey:            | ADUGONOVZSGHBC-UHFFFAOYSA-N                              |
| Formula:             | C9H16O2                                                  |
| SMILES:              | CCC1(C(=O)OC)CCCC1                                       |
| Mol. weight [g/mol]: | 156.22                                                   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -177.96 | kJ/mol  | Joback Method  |
| hf            | -398.17 | kJ/mol  | Joback Method  |
| hfus          | 9.49    | kJ/mol  | Joback Method  |
| hvap          | 43.89   | kJ/mol  | Joback Method  |
| log10ws       | -2.11   |         | Crippen Method |
| logp          | 2.130   |         | Crippen Method |
| mcvol         | 134.250 | ml/mol  | McGowan Method |
| pc            | 3049.04 | kPa     | Joback Method  |
| rinpol        | 1017.00 |         | NIST Webbook   |
| rinpol        | 1017.00 |         | NIST Webbook   |
| tb            | 497.13  | K       | Joback Method  |
| tc            | 706.51  | K       | Joback Method  |
| tf            | 298.15  | K       | Joback Method  |
| vc            | 0.502   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 308.52 | J/mol×K | 497.13          | Joback Method |
| cpg           | 324.57 | J/mol×K | 532.03          | Joback Method |
| cpg           | 339.62 | J/mol×K | 566.92          | Joback Method |
| cpg           | 353.78 | J/mol×K | 601.82          | Joback Method |
| cpg           | 367.14 | J/mol×K | 636.72          | Joback Method |
| cpg           | 379.79 | J/mol×K | 671.61          | Joback Method |
| cpg           | 391.83 | J/mol×K | 706.51          | 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>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=R164&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R164&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>rinpola:</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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