

# Cyclopropanecarboxamide

|                      |                                                   |
|----------------------|---------------------------------------------------|
| Other names:         | Cyclopropyl carboxamide<br>Carbamoylcyclopropane  |
| Inchi:               | InChI=1S/C4H7NO/c5-4(6)3-1-2-3/h3H,1-2H2,(H2,5,6) |
| InchiKey:            | AIMMVWEOZMVMS-UHFFFAOYSA-N                        |
| Formula:             | C4H7NO                                            |
| SMILES:              | NC(=O)C1CC1                                       |
| Mol. weight [g/mol]: | 85.10                                             |
| CAS:                 | 6228-73-5                                         |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -18.92  | kJ/mol  | Joback Method  |
| hf            | -131.88 | kJ/mol  | Joback Method  |
| hfus          | 11.05   | kJ/mol  | Joback Method  |
| hvap          | 41.80   | kJ/mol  | Joback Method  |
| log10ws       | -0.36   |         | Crippen Method |
| logp          | -0.118  |         | Crippen Method |
| mcvol         | 67.910  | ml/mol  | McGowan Method |
| pc            | 5470.75 | kPa     | Joback Method  |
| tb            | 424.06  | K       | Joback Method  |
| tc            | 636.48  | K       | Joback Method  |
| tf            | 285.97  | K       | Joback Method  |
| vc            | 0.252   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 135.59 | J/mol×K | 424.06          | Joback Method |
| cpg           | 144.85 | J/mol×K | 459.46          | Joback Method |
| cpg           | 153.49 | J/mol×K | 494.87          | Joback Method |
| cpg           | 161.54 | J/mol×K | 530.27          | Joback Method |
| cpg           | 169.04 | J/mol×K | 565.67          | Joback Method |
| cpg           | 176.03 | J/mol×K | 601.07          | Joback Method |
| cpg           | 182.54 | J/mol×K | 636.48          | 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=C6228735&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6228735&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>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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