

# Cyclopropanecarboxamide, N-n-propyl

|                      |                                                                      |
|----------------------|----------------------------------------------------------------------|
| Other names:         | N-Propylcyclopropanecarboxamide<br>Cyclopropanecarboxamide, N-propyl |
| Inchi:               | InChI=1S/C7H13NO/c1-2-5-8-7(9)6-3-4-6/h6H,2-5H2,1H3,(H,8,9)          |
| InchiKey:            | ATADNMCXCXUSOW-UHFFFAOYSA-N                                          |
| Formula:             | C7H13NO                                                              |
| SMILES:              | CCCNC(=O)C1CC1                                                       |
| Mol. weight [g/mol]: | 127.18                                                               |
| CAS:                 | 26389-59-3                                                           |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 29.28   | kJ/mol  | Joback Method  |
| hf            | -174.12 | kJ/mol  | Joback Method  |
| hfus          | 18.72   | kJ/mol  | Joback Method  |
| hvap          | 44.27   | kJ/mol  | Joback Method  |
| log10ws       | -1.37   |         | Crippen Method |
| logp          | 0.923   |         | Crippen Method |
| mcvol         | 110.180 | ml/mol  | McGowan Method |
| pc            | 3526.27 | kPa     | Joback Method  |
| rinpol        | 1197.00 |         | NIST Webbook   |
| tb            | 470.34  | K       | Joback Method  |
| tc            | 664.97  | K       | Joback Method  |
| tf            | 289.18  | K       | Joback Method  |
| vc            | 0.425   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 244.33 | J/mol×K | 470.34          | Joback Method |
| cpg           | 257.31 | J/mol×K | 502.78          | Joback Method |
| cpg           | 269.55 | J/mol×K | 535.22          | Joback Method |
| cpg           | 281.10 | J/mol×K | 567.65          | Joback Method |
| cpg           | 292.00 | J/mol×K | 600.09          | Joback Method |
| cpg           | 302.27 | J/mol×K | 632.53          | Joback Method |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C26389593&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26389593&amp;Units=SI</a> |
| Crippen Method: | <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>rinpol:</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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