

# Cyclopropanecarboxamide, N-(4-fluorophenyl)-

**Inchi:** InChI=1S/C10H10FNO/c11-8-3-5-9(6-4-8)12-10(13)7-1-2-7/h3-7H,1-2H2,(H,12,13)  
**InchiKey:** NLCQIPMGECDKHZ-UHFFFAOYSA-N  
**Formula:** C10H10FNO  
**SMILES:** O=C(Nc1ccc(F)cc1)C1CC1  
**Mol. weight [g/mol]:** 179.19

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -37.49  | kJ/mol  | Joback Method  |
| hf            | -207.09 | kJ/mol  | Joback Method  |
| hfus          | 23.22   | kJ/mol  | Joback Method  |
| hvap          | 53.07   | kJ/mol  | Joback Method  |
| log10ws       | -2.50   |         | Crippen Method |
| logp          | 2.174   |         | Crippen Method |
| mcvol         | 130.460 | ml/mol  | McGowan Method |
| pc            | 3456.14 | kPa     | Joback Method  |
| rinpol        | 1573.00 |         | NIST Webbook   |
| rinpol        | 1573.00 |         | NIST Webbook   |
| tb            | 569.91  | K       | Joback Method  |
| tc            | 790.97  | K       | Joback Method  |
| tf            | 362.52  | K       | Joback Method  |
| vc            | 0.503   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 316.96 | J/mol×K | 569.91          | Joback Method |
| cpg           | 330.44 | J/mol×K | 606.75          | Joback Method |
| cpg           | 342.95 | J/mol×K | 643.60          | Joback Method |
| cpg           | 354.54 | J/mol×K | 680.44          | Joback Method |
| cpg           | 365.28 | J/mol×K | 717.28          | Joback Method |
| cpg           | 375.24 | J/mol×K | 754.13          | Joback Method |
| cpg           | 384.47 | J/mol×K | 790.97          | 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=U307185&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307185&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>rlnpol:</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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