

# Cyclohexanecarboxamide, N-(4-fluorophenyl)-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C13H16FNO/c14-11-6-8-12(9-7-11)15-13(16)10-4-2-1-3-5-10/h6-10H,1-5H2,(H

RQMDSCPCNJHYJL-UHFFFAOYSA-N

C13H16FNO

O=C(Nc1ccc(F)cc1)C1CCCCC1

221.27

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -48.53  | kJ/mol  | Joback Method  |
| hf            | -287.49 | kJ/mol  | Joback Method  |
| hfus          | 24.69   | kJ/mol  | Joback Method  |
| hvap          | 60.26   | kJ/mol  | Joback Method  |
| log10ws       | -3.75   |         | Crippen Method |
| logp          | 3.344   |         | Crippen Method |
| mcvol         | 172.730 | ml/mol  | McGowan Method |
| pc            | 2729.71 | kPa     | Joback Method  |
| rinpol        | 1857.00 |         | NIST Webbook   |
| rinpol        | 1857.00 |         | NIST Webbook   |
| tb            | 651.36  | K       | Joback Method  |
| tc            | 882.32  | K       | Joback Method  |
| tf            | 385.77  | K       | Joback Method  |
| vc            | 0.647   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 469.15 | J/mol×K | 651.36          | Joback Method |
| cpg           | 486.86 | J/mol×K | 689.85          | Joback Method |
| cpg           | 503.26 | J/mol×K | 728.35          | Joback Method |
| cpg           | 518.41 | J/mol×K | 766.84          | Joback Method |
| cpg           | 532.36 | J/mol×K | 805.33          | Joback Method |
| cpg           | 545.16 | J/mol×K | 843.82          | Joback Method |
| cpg           | 556.88 | J/mol×K | 882.32          | 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=U306945&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U306945&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>                         |
| <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>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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