

# 3-Chloro-2-fluorobenzamide, N-pentyl-

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C12H15ClFNO/c1-2-3-4-8-15-12(16)9-6-5-7-10(13)11(9)14/h5-7H,2-4,8H2,1H3 |
| <b>InchiKey:</b>            | LFMPIITXVHOGLI-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C12H15ClFNO  |
| <b>SMILES:</b>              | CCCCCNC(=O)c1cccc(Cl)c1F   |
| <b>Mol. weight [g/mol]:</b> | 243.71   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -102.96 | kJ/mol               | Joback Method  |
| hf            | -348.38 | kJ/mol               | Joback Method  |
| hfus          | 34.07   | kJ/mol               | Joback Method  |
| hvap          | 62.66   | kJ/mol               | Joback Method  |
| log10ws       | -4.51   |                      | Crippen Method |
| logp          | 3.399   |                      | Crippen Method |
| mcvol         | 181.740 | ml/mol               | McGowan Method |
| pc            | 2322.54 | kPa                  | Joback Method  |
| rinpola       | 1906.00 |                      | NIST Webbook   |
| rinpola       | 1906.00 |                      | NIST Webbook   |
| tb            | 651.34  | K                    | Joback Method  |
| tc            | 855.88  | K                    | Joback Method  |
| tf            | 409.56  | K                    | Joback Method  |
| vc            | 0.708   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 454.02 | J/molxK | 651.34          | Joback Method |
| cpg           | 467.16 | J/molxK | 685.43          | Joback Method |
| cpg           | 479.52 | J/molxK | 719.52          | Joback Method |
| cpg           | 491.12 | J/molxK | 753.61          | Joback Method |
| cpg           | 501.99 | J/molxK | 787.70          | Joback Method |
| cpg           | 512.16 | J/molxK | 821.79          | Joback Method |
| cpg           | 521.65 | J/molxK | 855.88          | 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=U358131&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358131&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>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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