

# Benzamide, 3-fluoro-4-trifluoromethyl-N-isobutyl-

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C12H13F4NO/c1-7(2)6-17-11(18)8-3-4-9(10(13)5-8)12(14,15)16/h3-5,7H,6H2, |
| <b>InchiKey:</b>            | NDAAFAXSTNFSOR-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C12H13F4NO   |
| <b>SMILES:</b>              | CC(C)CNC(=O)c1ccc(C(F)(F)F)c(F)c1  |
| <b>Mol. weight [g/mol]:</b> | 263.23   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -675.06 | kJ/mol               | Joback Method  |
| hf            | -935.00 | kJ/mol               | Joback Method  |
| hfus          | 28.18   | kJ/mol               | Joback Method  |
| hvap          | 54.14   | kJ/mol               | Joback Method  |
| log10ws       | -4.27   |                      | Crippen Method |
| logp          | 3.230   |                      | Crippen Method |
| mvol          | 174.810 | ml/mol               | McGowan Method |
| pc            | 2171.40 | kPa                  | Joback Method  |
| rinpol        | 1553.00 |                      | NIST Webbook   |
| rinpol        | 1553.00 |                      | NIST Webbook   |
| tb            | 608.05  | K                    | Joback Method  |
| tc            | 797.38  | K                    | Joback Method  |
| tf            | 368.83  | K                    | Joback Method  |
| vc            | 0.696   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 455.31 | J/mol×K | 608.05          | Joback Method |
| cpg           | 468.42 | J/mol×K | 639.60          | Joback Method |
| cpg           | 480.73 | J/mol×K | 671.16          | Joback Method |
| cpg           | 492.26 | J/mol×K | 702.71          | Joback Method |
| cpg           | 503.05 | J/mol×K | 734.27          | Joback Method |
| cpg           | 513.14 | J/mol×K | 765.82          | Joback Method |
| cpg           | 522.58 | J/mol×K | 797.38          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <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=U407885&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407885&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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