# Benzamide, 3-trifluoromethyl-2-fluoro-N-(3-trifluoromethyl-2-fl

**Inchi:** InChI=1S/C21H17F8NO2/c1-11(2)9-10-30(18(31)12-5-3-7-14(16(12)22)20(24,25)26)19(3

**InchiKey:** NSSDDGLINYWGEZ-UHFFFAOYSA-N

**Formula:** C21H17F8NO2

**SMILES:** CC(C)CCN(C(=O)c1cccc(C(F)(F)F)c1F)C(=O)c1cccc(C(F)(F)F)c1F

**Mol. weight [g/mol]:** 467.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1390.06 | kJ/mol | Joback Method |
| hf | -1798.88 | kJ/mol | Joback Method |
| hfus | 49.18 | kJ/mol | Joback Method |
| hvap | 75.56 | kJ/mol | Joback Method |
| log10ws | -7.89 | | Crippen Method |
| logp | 6.331 | | Crippen Method |
| mcvol | 286.510 | ml/mol | McGowan Method |
| pc | 1255.70 | kPa | Joback Method |
| rinpol | 1995.00 | | NIST Webbook |
| rinpol | 1995.00 | | NIST Webbook |
| tb | 860.60 | K | Joback Method |
| tc | 1059.97 | K | Joback Method |
| tf | 556.24 | K | Joback Method |
| vc | 1.141 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 883.75 | J/mol×K | 860.60 | Joback Method |
| cpg | 895.99 | J/mol×K | 893.83 | Joback Method |
| cpg | 907.36 | J/mol×K | 927.06 | Joback Method |
| cpg | 917.92 | J/mol×K | 960.29 | Joback Method |
| cpg | 927.78 | J/mol×K | 993.52 | Joback Method |
| cpg | 937.02 | J/mol×K | 1026.75 | Joback Method |
| cpg | 945.73 | J/mol×K | 1059.97 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407721&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |