# Benzamide, 2-trifluoromethyl-5-fluoro-N-ethyl-

**Inchi:** InChI=1S/C10H9F4NO/c1-2-15-9(16)7-5-6(11)3-4-8(7)10(12,13)14/h3-5H,2H2,1H3,(H,15
**InchiKey:** VNEXYWWWVPOOCL-UHFFFAOYSA-N
**Formula:** C10H9F4NO
**SMILES:** CCNC(=O)c1cc(F)ccc1C(F)(F)F
**Mol. weight [g/mol]:** 235.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -689.46 | kJ/mol | Joback Method |
| hf | -888.44 | kJ/mol | Joback Method |
| hfus | 26.52 | kJ/mol | Joback Method |
| hvap | 50.07 | kJ/mol | Joback Method |
| log10ws | -3.67 | | Crippen Method |
| logp | 2.594 | | Crippen Method |
| mcvol | 146.630 | ml/mol | McGowan Method |
| pc | 2597.78 | kPa | Joback Method |
| rinpol | 1357.00 | | NIST Webbook |
| tb | 562.73 | K | Joback Method |
| tc | 752.89 | K | Joback Method |
| tf | 361.29 | K | Joback Method |
| vc | 0.590 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 359.53 | J/mol×K | 562.73 | Joback Method |
| cpg | 371.10 | J/mol×K | 594.42 | Joback Method |
| cpg | 381.94 | J/mol×K | 626.12 | Joback Method |
| cpg | 392.07 | J/mol×K | 657.81 | Joback Method |
| cpg | 401.54 | J/mol×K | 689.50 | Joback Method |
| cpg | 410.38 | J/mol×K | 721.20 | Joback Method |
| cpg | 418.63 | J/mol×K | 752.89 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407673&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |