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

**Inchi:** InChI=1S/C20H29F4NO/c1-2-3-4-5-6-7-8-9-10-11-14-25-19(26)16-12-13-17(18(21)15-16

**InchiKey:** LNZZXIYKEWPTFP-UHFFFAOYSA-N

**Formula:** C20H29F4NO

**SMILES:** CCCCCCCCCCCCNC(=O)c1ccc(C(F)(F)F)c(F)c1

**Mol. weight [g/mol]:** 375.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -605.26 | kJ/mol | Joback Method |
| hf | -1094.84 | kJ/mol | Joback Method |
| hfus | 52.42 | kJ/mol | Joback Method |
| hvap | 72.33 | kJ/mol | Joback Method |
| log10ws | -7.86 | | Crippen Method |
| logp | 6.495 | | Crippen Method |
| mcvol | 287.530 | ml/mol | McGowan Method |
| pc | 1171.22 | kPa | Joback Method |
| rinpol | 2399.00 | | NIST Webbook |
| rinpol | 2399.00 | | NIST Webbook |
| tb | 791.53 | K | Joback Method |
| tc | 975.67 | K | Joback Method |
| tf | 473.99 | K | Joback Method |
| vc | 1.149 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 888.97 | J/mol×K | 791.53 | Joback Method |
| cpg | 905.14 | J/mol×K | 822.22 | Joback Method |
| cpg | 920.39 | J/mol×K | 852.91 | Joback Method |
| cpg | 934.76 | J/mol×K | 883.60 | Joback Method |
| cpg | 948.30 | J/mol×K | 914.29 | Joback Method |
| cpg | 961.08 | J/mol×K | 944.98 | Joback Method |
| cpg | 973.13 | J/mol×K | 975.67 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407897&Units=SI |

# 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 |