# Benzamide, 2-fluoro-3-trifluoromethyl-N-pentyl-N-dodecyl-

**Inchi:** InChI=1S/C25H39F4NO/c1-3-5-7-8-9-10-11-12-13-15-20-30(19-14-6-4-2)24(31)21-17-16

**InchiKey:** LOMJLKIUCCLNRK-UHFFFAOYSA-N

**Formula:** C25H39F4NO

**SMILES:** CCCCCCCCCCCCN(CCCCC)C(=O)c1cccc(C(F)(F)F)c1F

**Mol. weight [g/mol]:** 445.58

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -541.77 | kJ/mol | Joback Method |
| hf | -1183.98 | kJ/mol | Joback Method |
| hfus | 63.29 | kJ/mol | Joback Method |
| hvap | 79.07 | kJ/mol | Joback Method |
| log10ws | -9.33 | | Crippen Method |
| logp | 8.398 | | Crippen Method |
| mcvol | 357.980 | ml/mol | McGowan Method |
| pc | 856.47 | kPa | Joback Method |
| rinpol | 3202.00 | | NIST Webbook |
| tb | 868.20 | K | Joback Method |
| tc | 1062.93 | K | Joback Method |
| tf | 510.15 | K | Joback Method |
| vc | 1.413 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1170.73 | J/mol×K | 868.20 | Joback Method |
| cpg | 1189.72 | J/mol×K | 900.65 | Joback Method |
| cpg | 1207.60 | J/mol×K | 933.11 | Joback Method |
| cpg | 1224.45 | J/mol×K | 965.56 | Joback Method |
| cpg | 1240.35 | J/mol×K | 998.02 | Joback Method |
| cpg | 1255.39 | J/mol×K | 1030.47 | Joback Method |
| cpg | 1269.63 | J/mol×K | 1062.93 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U416700&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 |

# 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 |