# 3-Fluoro-6-trifluoromethylbenzamide, N-(3-methylphenyl)-

**Inchi:** InChI=1S/C15H11F4NO/c1-9-3-2-4-11(7-9)20-14(21)12-8-10(16)5-6-13(12)15(17,18)19/h
**InchiKey:** RJPZSTXMXCOTPJ-UHFFFAOYSA-N
**Formula:** C15H11F4NO
**SMILES:** Cc1cccc(NC(=O)c2cc(F)ccc2C(F)(F)F)c1
**Mol. weight [g/mol]:** 297.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -544.58 | kJ/mol | Joback Method |
| hf | -766.58 | kJ/mol | Joback Method |
| hfus | 33.12 | kJ/mol | Joback Method |
| hvap | 64.14 | kJ/mol | Joback Method |
| log10ws | -5.36 | | Crippen Method |
| logp | 4.405 | | Crippen Method |
| mcvol | 193.320 | ml/mol | McGowan Method |
| pc | 2212.45 | kPa | Joback Method |
| rinpol | 1932.00 | | NIST Webbook |
| rinpol | 1932.00 | | NIST Webbook |
| tb | 708.79 | K | Joback Method |
| tc | 922.89 | K | Joback Method |
| tf | 456.58 | K | Joback Method |
| vc | 0.761 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 524.18 | J/mol×K | 708.79 | Joback Method |
| cpg | 536.84 | J/mol×K | 744.47 | Joback Method |
| cpg | 548.52 | J/mol×K | 780.16 | Joback Method |
| cpg | 559.28 | J/mol×K | 815.84 | Joback Method |
| cpg | 569.18 | J/mol×K | 851.52 | Joback Method |
| cpg | 578.30 | J/mol×K | 887.21 | Joback Method |
| cpg | 586.70 | J/mol×K | 922.89 | Joback Method |

# Sources

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|---|---|
| **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=U358077&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |