# m-(trifluoromethyl)benzamide

**Other names:** 3-CF3-C6H4CONH2
**Inchi:** InChI=1S/C8H6F3NO/c9-8(10,11)6-3-1-2-5(4-6)7(12)13/h1-4H,(H2,12,13)
**InchiKey:** XBGXGCOLWCMVOI-UHFFFAOYSA-N
**Formula:** C8H6F3NO
**SMILES:** NC(=O)c1cccc(C(F)(F)F)c1
**Mol. weight [g/mol]:** 189.13
**CAS:** 1801-10-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 866.90 | kJ/mol | NIST Webbook |
| basg | 836.00 | kJ/mol | NIST Webbook |
| gf | -524.80 | kJ/mol | Joback Method |
| hf | -659.26 | kJ/mol | Joback Method |
| hfus | 18.75 | kJ/mol | Joback Method |
| hvap | 49.98 | kJ/mol | Joback Method |
| log10ws | -2.75 | | Crippen Method |
| logp | 1.804 | | Crippen Method |
| mcvol | 116.680 | ml/mol | McGowan Method |
| pc | 3602.88 | kPa | Joback Method |
| tb | 535.08 | K | Joback Method |
| tc | 748.18 | K | Joback Method |
| tf | 356.24 | K | Joback Method |
| vc | 0.454 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 271.67 | J/mol×K | 535.08 | Joback Method |
| cpg | 282.12 | J/mol×K | 570.60 | Joback Method |
| cpg | 291.77 | J/mol×K | 606.11 | Joback Method |
| cpg | 300.65 | J/mol×K | 641.63 | Joback Method |
| cpg | 308.81 | J/mol×K | 677.15 | Joback Method |
| cpg | 316.31 | J/mol×K | 712.67 | Joback Method |

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|---|---|---|---|---|
| cpg | 323.18 | J/mol×K | 748.18 | 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=C1801101&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |