# 1-Fluoro-3-(trifluoro-methyl)benzene

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|---|---|
| **Other names:** | m-Fluorobenzotrifluoride |
| | 3-Fluorobenzotrifluoride |
| | Benzene, 1-fluoro-3-(trifluoromethyl)- |
| | m,«alpha»,«alpha»,«alpha»-Tetrafluorotoluene |
| | Toluene, «alpha»,«alpha»,«alpha»-m-tetrafluoro- |
| | Toluene, m,«alpha»,«alpha»,«alpha»-tetrafluoro- |
| | Trifluoromethyl-3-fluorobenzene |
| | 1-(Trifluoromethyl)-3-fluorobenzene |
| | m,alpha,alpha,alpha-Tetrafluorotoluene |
| | 3-Fluoro(trifluoromethyl)benzene |
| | «alpha»,«alpha»,«alpha»,3-Tetrafluorotoluene |
| **Inchi:** | InChI=1S/C7H4F4/c8-6-3-1-2-5(4-6)7(9,10)11/h1-4H |
| **InchiKey:** | GBOWGKOVMBDPJF-UHFFFAOYSA-N |
| **Formula:** | C7H4F4 |
| **SMILES:** | Fc1cccc(C(F)(F)F)c1 |
| **Mol. weight [g/mol]:** | 164.10 |
| **CAS:** | 401-80-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -3211.70 ± 0.59 | kJ/mol | NIST Webbook |
| gf | -665.56 | kJ/mol | Joback Method |
| hf | -792.20 ± 1.10 | kJ/mol | NIST Webbook |
| hfl | -830.20 ± 1.10 | kJ/mol | NIST Webbook |
| hfus | 12.44 | kJ/mol | Joback Method |
| hvap | 37.90 ± 0.20 | kJ/mol | NIST Webbook |
| log10ws | -2.91 | | Crippen Method |
| logp | 2.845 | | Crippen Method |
| mcvol | 92.810 | ml/mol | McGowan Method |
| pc | 3322.01 | kPa | Joback Method |
| rinpol | 861.00 | | NIST Webbook |
| rinpol | 861.00 | | NIST Webbook |
| rinpol | 861.00 | | NIST Webbook |
| tb | 374.70 | K | NIST Webbook |
| tb | 373.00 | K | NIST Webbook |
| tc | 566.36 | K | Joback Method |
| tf | 212.37 | K | Joback Method |

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|---|---|---|---|
| vc | 0.381 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 219.11 | J/mol×K | 536.14 | Joback Method |
| cpg | 174.38 | J/mol×K | 385.07 | Joback Method |
| cpg | 184.55 | J/mol×K | 415.28 | Joback Method |
| cpg | 194.08 | J/mol×K | 445.50 | Joback Method |
| cpg | 203.00 | J/mol×K | 475.71 | Joback Method |
| cpg | 211.34 | J/mol×K | 505.93 | Joback Method |
| cpg | 226.36 | J/mol×K | 566.36 | Joback Method |
| hvapt | 36.80 | kJ/mol | 361.50 | NIST Webbook |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C401809&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

**chl:** Standard liquid enthalpy of combustion
**cpg:** Ideal gas heat capacity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfl:** Liquid phase enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**hvapt:** Enthalpy of vaporization at a given temperature
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume

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|---|---|
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |