# Trifluoroacetamide, N-[1-(3-methoxyphenyl)ethyl]

**Inchi:** InChI=1S/C9H8F3NO2/c1-15-7-4-2-3-6(5-7)13-8(14)9(10,11)12/h2-5H,1H3,(H,13,14)
**InchiKey:** TZCQPHOSHKXEQV-UHFFFAOYSA-N
**Formula:** C9H8F3NO2
**SMILES:** COc1cccc(NC(=O)C(F)(F)F)c1
**Mol. weight [g/mol]:** 219.16

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -598.44 | kJ/mol | Joback Method |
| hf | -792.44 | kJ/mol | Joback Method |
| hfus | 22.43 | kJ/mol | Joback Method |
| hvap | 50.41 | kJ/mol | Joback Method |
| log10ws | -2.46 | | Crippen Method |
| logp | 2.196 | | Crippen Method |
| mcvol | 136.640 | ml/mol | McGowan Method |
| pc | 3009.03 | kPa | Joback Method |
| rinpol | 1431.00 | | NIST Webbook |
| rinpol | 1431.00 | | NIST Webbook |
| tb | 558.02 | K | Joback Method |
| tc | 757.27 | K | Joback Method |
| tf | 359.14 | K | Joback Method |
| vc | 0.533 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 329.61 | J/mol×K | 558.02 | Joback Method |
| cpg | 340.98 | J/mol×K | 591.23 | Joback Method |
| cpg | 351.60 | J/mol×K | 624.44 | Joback Method |
| cpg | 361.52 | J/mol×K | 657.64 | Joback Method |
| cpg | 370.75 | J/mol×K | 690.85 | Joback Method |
| cpg | 379.33 | J/mol×K | 724.06 | Joback Method |
| cpg | 387.29 | J/mol×K | 757.27 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R74056&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |