# Methyl 3-(N-trifluoroacetylamino)benzoate

**Inchi:** InChI=1S/C10H8F3NO3/c1-17-8(15)6-3-2-4-7(5-6)14-9(16)10(11,12)13/h2-5H,1H3,(H,14
**InchiKey:** KZAHZSHFBNWZPX-UHFFFAOYSA-N
**Formula:** C10H8F3NO3
**SMILES:** COC(=O)c1cccc(NC(=O)C(F)(F)F)c1
**Mol. weight [g/mol]:** 247.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -718.94 | kJ/mol | Joback Method |
| hf | -925.66 | kJ/mol | Joback Method |
| hfus | 26.62 | kJ/mol | Joback Method |
| hvap | 59.38 | kJ/mol | Joback Method |
| log10ws | -2.58 | | Crippen Method |
| logp | 1.974 | | Crippen Method |
| mcvol | 152.300 | ml/mol | McGowan Method |
| pc | 2902.98 | kPa | Joback Method |
| rinpol | 1529.00 | | NIST Webbook |
| rinpol | 1529.00 | | NIST Webbook |
| tb | 634.77 | K | Joback Method |
| tc | 838.61 | K | Joback Method |
| tf | 420.34 | K | Joback Method |
| vc | 0.596 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 390.09 | J/mol×K | 634.77 | Joback Method |
| cpg | 400.83 | J/mol×K | 668.74 | Joback Method |
| cpg | 410.79 | J/mol×K | 702.72 | Joback Method |
| cpg | 420.01 | J/mol×K | 736.69 | Joback Method |
| cpg | 428.52 | J/mol×K | 770.67 | Joback Method |
| cpg | 436.34 | J/mol×K | 804.64 | Joback Method |
| cpg | 443.53 | J/mol×K | 838.61 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U374362&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |