# 2,3,4-Trifluorobenzoic acid, ethyl ester

**Other names:** Ethyl 2,3,4-trifluorobenzoate
**Inchi:** InChI=1S/C9H7F3O2/c1-2-14-9(13)5-3-4-6(10)8(12)7(5)11/h3-4H,2H2,1H3
**InchiKey:** MLANUBGYWOMWLZ-UHFFFAOYSA-N
**Formula:** C9H7F3O2
**SMILES:** CCOC(=O)c1ccc(F)c(F)c1F
**Mol. weight [g/mol]:** 204.15
**CAS:** 351354-50-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -709.93 | kJ/mol | Joback Method |
| hf | -860.10 | kJ/mol | Joback Method |
| hfus | 23.97 | kJ/mol | Joback Method |
| hvap | 46.59 | kJ/mol | Joback Method |
| log10ws | -3.13 | | Crippen Method |
| logp | 2.281 | | Crippen Method |
| mcvol | 126.660 | ml/mol | McGowan Method |
| pc | 2814.34 | kPa | Joback Method |
| rinpol | 1154.00 | | NIST Webbook |
| rinpol | 1154.00 | | NIST Webbook |
| tb | 521.04 | K | Joback Method |
| tc | 709.89 | K | Joback Method |
| tf | 329.10 | K | Joback Method |
| vc | 0.509 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 280.60 | J/mol×K | 521.04 | Joback Method |
| cpg | 290.49 | J/mol×K | 552.51 | Joback Method |
| cpg | 299.95 | J/mol×K | 583.99 | Joback Method |
| cpg | 308.98 | J/mol×K | 615.46 | Joback Method |
| cpg | 317.58 | J/mol×K | 646.94 | Joback Method |
| cpg | 325.75 | J/mol×K | 678.41 | Joback Method |

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|---|---|---|---|---|
| cpg | 333.50 | J/mol×K | 709.89 | 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=C351354502&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 |