# Terephthalic acid, methyl 2,3,4-trifluorophenyl ester

**Inchi:** InChI=1S/C15H9F3O4/c1-21-14(19)8-2-4-9(5-3-8)15(20)22-11-7-6-10(16)12(17)13(11)18

**InchiKey:** QRBPJEAKFBBPQY-UHFFFAOYSA-N

**Formula:** C15H9F3O4

**SMILES:** COC(=O)c1ccc(C(=O)Oc2ccc(F)c(F)c2F)cc1

**Mol. weight [g/mol]:** 310.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -790.55 | kJ/mol | Joback Method |
| hf | -1003.68 | kJ/mol | Joback Method |
| hfus | 35.95 | kJ/mol | Joback Method |
| hvap | 72.05 | kJ/mol | Joback Method |
| log10ws | -4.80 | | Crippen Method |
| logp | 3.110 | | Crippen Method |
| mcvol | 194.880 | ml/mol | McGowan Method |
| pc | 2269.73 | kPa | Joback Method |
| rinpol | 2249.00 | | NIST Webbook |
| tb | 766.27 | K | Joback Method |
| tc | 981.75 | K | Joback Method |
| tf | 507.82 | K | Joback Method |
| vc | 0.761 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 524.16 | J/mol×K | 766.27 | Joback Method |
| cpg | 535.31 | J/mol×K | 802.18 | Joback Method |
| cpg | 545.53 | J/mol×K | 838.10 | Joback Method |
| cpg | 554.83 | J/mol×K | 874.01 | Joback Method |
| cpg | 563.22 | J/mol×K | 909.92 | Joback Method |
| cpg | 570.69 | J/mol×K | 945.83 | Joback Method |
| cpg | 577.25 | J/mol×K | 981.75 | 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=U415798&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 |