# methyl 3,4,5-trimethylbenzoate

**Inchi:** InChI=1S/C11H14O2/c1-7-5-10(11(12)13-4)6-8(2)9(7)3/h5-6H,1-4H3
**InchiKey:** MMOVUCSZRKTFNP-UHFFFAOYSA-N
**Formula:** C11H14O2
**SMILES:** COC(=O)c1cc(C)c(C)c(C)c1
**Mol. weight [g/mol]:** 178.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -108.66 | kJ/mol | Joback Method |
| hf | -313.05 | kJ/mol | Joback Method |
| hfus | 19.91 | kJ/mol | Joback Method |
| hvap | 53.50 | kJ/mol | Joback Method |
| log10ws | -3.14 | | Crippen Method |
| logp | 2.398 | | Crippen Method |
| mcvol | 149.530 | ml/mol | McGowan Method |
| pc | 2651.56 | kPa | Joback Method |
| rinpol | 1671.00 | | NIST Webbook |
| tb | 568.99 | K | Joback Method |
| tc | 781.39 | K | Joback Method |
| tf | 349.87 | K | Joback Method |
| vc | 0.568 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 345.39 | J/mol×K | 568.99 | Joback Method |
| cpg | 406.88 | J/mol×K | 745.99 | Joback Method |
| cpg | 395.89 | J/mol×K | 710.59 | Joback Method |
| cpg | 384.25 | J/mol×K | 675.19 | Joback Method |
| cpg | 371.96 | J/mol×K | 639.79 | Joback Method |
| cpg | 359.01 | J/mol×K | 604.39 | Joback Method |
| cpg | 417.21 | J/mol×K | 781.39 | Joback Method |
| dvisc | 0.0001868 | Pa×s | 568.99 | Joback Method |
| dvisc | 0.0002264 | Pa×s | 532.47 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002823 | Pa×s | 495.95 | Joback Method |
| dvisc | 0.0003644 | Pa×s | 459.43 | Joback Method |
| dvisc | 0.0004918 | Pa×s | 422.91 | Joback Method |
| dvisc | 0.0007022 | Pa×s | 386.39 | Joback Method |
| dvisc | 0.0010802 | Pa×s | 349.87 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R218801&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |

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