# 4-Methylbenzoic acid, 2,2,2-trichloroethyl ester

**Inchi:** InChI=1S/C10H9Cl3O2/c1-7-2-4-8(5-3-7)9(14)15-6-10(11,12)13/h2-5H,6H2,1H3
**InchiKey:** NSEMXPHSOPXKLU-UHFFFAOYSA-N
**Formula:** C10H9Cl3O2
**SMILES:** Cc1ccc(C(=O)OCC(Cl)(Cl)Cl)cc1
**Mol. weight [g/mol]:** 267.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -130.77 | kJ/mol | Joback Method |
| hf | -325.44 | kJ/mol | Joback Method |
| hfus | 23.27 | kJ/mol | Joback Method |
| hvap | 61.81 | kJ/mol | Joback Method |
| log10ws | -4.17 | | Crippen Method |
| logp | 3.522 | | Crippen Method |
| mcvol | 172.160 | ml/mol | McGowan Method |
| pc | 2746.90 | kPa | Joback Method |
| rinpol | 1731.00 | | NIST Webbook |
| rinpol | 1731.00 | | NIST Webbook |
| tb | 645.21 | K | Joback Method |
| tc | 884.19 | K | Joback Method |
| tf | 405.74 | K | Joback Method |
| vc | 0.647 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 376.75 | J/mol×K | 645.21 | Joback Method |
| cpg | 387.87 | J/mol×K | 685.04 | Joback Method |
| cpg | 398.05 | J/mol×K | 724.87 | Joback Method |
| cpg | 407.37 | J/mol×K | 764.70 | Joback Method |
| cpg | 415.86 | J/mol×K | 804.53 | Joback Method |
| cpg | 423.59 | J/mol×K | 844.36 | Joback Method |
| cpg | 430.61 | J/mol×K | 884.19 | Joback Method |
| dvisc | 0.0013925 | Pa×s | 405.74 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0008277 | Pa×s | 445.65 | Joback Method |
| dvisc | 0.0005359 | Pa×s | 485.56 | Joback Method |
| dvisc | 0.0003706 | Pa×s | 525.48 | Joback Method |
| dvisc | 0.0002700 | Pa×s | 565.39 | Joback Method |
| dvisc | 0.0002051 | Pa×s | 605.30 | Joback Method |
| dvisc | 0.0001612 | Pa×s | 645.21 | Joback Method |

# Sources

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|---|---|
| **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=U354153&Units=SI |

# Legend

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