# Monomethyl 2,3,5,6-tetrachloroterephthalate

| | |
|---|---|
| **Other names:** | 1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-, monomethyl ester |
| | Terephthalic acid, tetrachloro-, monomethyl ester |
| | Dacthal monoacid |
| | Methyl 2,3,5,6-tetrachloroterephthalate |
| | Monomethyl tetrachloroterephthalate |
| | Tetrachloroterephthalic acid methyl ester |
| | Tetrachloroterephthalic acid, monomethyl ester |
| | 2,3,5,6-Tetrachloro-4-(methoxycarbonyl)benzoic acid |
| | Chlorthal monomethyl |
| | 1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-, 4-methyl ester |
| | Methyl tetrachloroterephthalic acid ester |
| **Inchi:** | InChI=1S/C9H4Cl4O4/c1-17-9(16)3-6(12)4(10)2(8(14)15)5(11)7(3)13/h1H3,(H,14,15) |
| **InchiKey:** | SXINVWXSZUQKSW-UHFFFAOYSA-N |
| **Formula:** | C9H4Cl4O4 |
| **SMILES:** | COC(=O)c1c(Cl)c(Cl)c(C(=O)O)c(Cl)c1Cl |
| **Mol. weight [g/mol]:** | 317.94 |
| **CAS:** | 887-54-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -458.22 | kJ/mol | Joback Method |
| hf | -622.48 | kJ/mol | Joback Method |
| hfus | 36.42 | kJ/mol | Joback Method |
| hvap | 91.33 | kJ/mol | Joback Method |
| log10ws | -4.51 | | Crippen Method |
| logp | 3.785 | | Crippen Method |
| mcvol | 177.750 | ml/mol | McGowan Method |
| pc | 3181.14 | kPa | Joback Method |
| tb | 828.96 | K | Joback Method |
| tc | 1053.81 | K | Joback Method |
| tf | 444.86 ± 0.20 | K | NIST Webbook |
| tf | 450.50 ± 0.20 | K | NIST Webbook |
| vc | 0.676 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 377.83 | J/mol×K | 828.96 | Joback Method |
| cpg | 383.33 | J/mol×K | 866.43 | Joback Method |
| cpg | 388.26 | J/mol×K | 903.91 | Joback Method |
| cpg | 392.60 | J/mol×K | 941.38 | Joback Method |
| cpg | 396.36 | J/mol×K | 978.86 | Joback Method |
| cpg | 399.51 | J/mol×K | 1016.33 | Joback Method |
| cpg | 402.05 | J/mol×K | 1053.81 | Joback Method |
| dvisc | 0.0002483 | Pa×s | 582.80 | Joback Method |
| dvisc | 0.0001589 | Pa×s | 623.83 | Joback Method |
| dvisc | 0.0001075 | Pa×s | 664.85 | Joback Method |
| dvisc | 0.0000760 | Pa×s | 705.88 | Joback Method |
| dvisc | 0.0000559 | Pa×s | 746.91 | Joback Method |
| dvisc | 0.0000424 | Pa×s | 787.93 | Joback Method |
| dvisc | 0.0000331 | Pa×s | 828.96 | Joback Method |
| hfust | 16.89 | kJ/mol | 444.30 | NIST Webbook |

# Sources

**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=C887547&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# 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
**hfust:** Enthalpy of fusion at a given temperature
**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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |