# 2,3,4,5-Tetramethylbenzoic acid

**Inchi:** InChI=1S/C11H14O2/c1-6-5-10(11(12)13)9(4)8(3)7(6)2/h5H,1-4H3,(H,12,13)
**InchiKey:** JEBOPSGVIIUIQD-UHFFFAOYSA-N
**Formula:** C11H14O2
**SMILES:** Cc1cc(C(=O)O)c(C)c(C)c1C
**Mol. weight [g/mol]:** 178.23
**CAS:** 2529-39-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -150.11 | kJ/mol | Joback Method |
| hf | -398.70 ± 2.30 | kJ/mol | NIST Webbook |
| hfs | -514.60 ± 2.20 | kJ/mol | NIST Webbook |
| hfus | 22.42 | kJ/mol | Joback Method |
| hsub | 115.90 ± 0.60 | kJ/mol | NIST Webbook |
| hsub | 115.90 | kJ/mol | NIST Webbook |
| hsub | 115.90 ± 0.60 | kJ/mol | NIST Webbook |
| hvap | 68.43 | kJ/mol | Joback Method |
| log10ws | -3.43 | | Crippen Method |
| logp | 2.618 | | Crippen Method |
| mcvol | 149.530 | ml/mol | McGowan Method |
| pc | 2928.17 | kPa | Joback Method |
| tb | 643.73 | K | Joback Method |
| tc | 844.89 | K | Joback Method |
| tf | 400.98 | K | Joback Method |
| vc | 0.569 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 371.49 | J/mol×K | 643.73 | Joback Method |
| cpg | 382.80 | J/mol×K | 677.26 | Joback Method |
| cpg | 393.53 | J/mol×K | 710.78 | Joback Method |
| cpg | 403.70 | J/mol×K | 744.31 | Joback Method |
| cpg | 413.31 | J/mol×K | 777.84 | Joback Method |

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|---|---|---|---|---|
| cpg | 422.39 | J/mol×K | 811.36 | Joback Method |
| cpg | 430.93 | J/mol×K | 844.89 | Joback Method |
| cps | 249.50 | J/mol×K | 298.15 | NIST Webbook |
| dvisc | 0.0013439 | Pa×s | 400.98 | Joback Method |
| dvisc | 0.0006556 | Pa×s | 441.44 | Joback Method |
| dvisc | 0.0003608 | Pa×s | 481.90 | Joback Method |
| dvisc | 0.0002178 | Pa×s | 522.36 | Joback Method |
| dvisc | 0.0001414 | Pa×s | 562.81 | Joback Method |
| dvisc | 0.0000972 | Pa×s | 603.27 | Joback Method |
| dvisc | 0.0000701 | Pa×s | 643.73 | Joback Method |
| hsubt | 113.40 ± 0.60 | kJ/mol | 348.50 | NIST Webbook |

# 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=C2529397&Units=SI

# Legend

**cpg:** Ideal gas heat capacity
**cps:** Solid phase heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfs:** Solid phase enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hsub:** Enthalpy of sublimation at standard conditions
**hsubt:** Enthalpy of sublimation 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