# Pentanedioic acid, 3,3-dimethyl-, dimethyl ester

**Other names:** Glutaric acid, 3,3-dimethyl-, dimethyl ester
Methyl 3,3-dimethylglutarate

**Inchi:** InChI=1S/C9H16O4/c1-9(2,5-7(10)12-3)6-8(11)13-4/h5-6H2,1-4H3

**InchiKey:** NPEAPWIQJBAJIO-UHFFFAOYSA-N

**Formula:** C9H16O4

**SMILES:** COC(=O)CC(C)(C)CC(=O)OC

**Mol. weight [g/mol]:** 188.22

**CAS:** 19184-67-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -440.10 | kJ/mol | Joback Method |
| hf | -727.44 | kJ/mol | Joback Method |
| hfus | 17.23 | kJ/mol | Joback Method |
| hvap | 52.64 | kJ/mol | Joback Method |
| log10ws | -1.07 | | Crippen Method |
| logp | 1.139 | | Crippen Method |
| mcvol | 152.550 | ml/mol | McGowan Method |
| pc | 2574.11 | kPa | Joback Method |
| tb | 554.67 | K | Joback Method |
| tc | 746.71 | K | Joback Method |
| tf | 337.93 | K | Joback Method |
| vc | 0.577 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 371.44 | J/mol×K | 554.67 | Joback Method |
| cpg | 384.56 | J/mol×K | 586.68 | Joback Method |
| cpg | 397.05 | J/mol×K | 618.68 | Joback Method |
| cpg | 408.91 | J/mol×K | 650.69 | Joback Method |
| cpg | 420.16 | J/mol×K | 682.69 | Joback Method |
| cpg | 430.80 | J/mol×K | 714.70 | Joback Method |
| cpg | 440.85 | J/mol×K | 746.71 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0022755 | Pa×s | 337.93 | Joback Method |
| dvisc | 0.0012362 | Pa×s | 374.05 | Joback Method |
| dvisc | 0.0007478 | Pa×s | 410.18 | Joback Method |
| dvisc | 0.0004907 | Pa×s | 446.30 | Joback Method |
| dvisc | 0.0003430 | Pa×s | 482.42 | Joback Method |
| dvisc | 0.0002520 | Pa×s | 518.55 | Joback Method |
| dvisc | 0.0001927 | Pa×s | 554.67 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 376.70 | K | 2.00 | 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=C19184679&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
**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
**tbrp:** Boiling point at reduced pressure

| | |
|---|---|
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |