# 2-Oxo-hexanedioic acid 1-methyl ester

**Inchi:** InChI=1S/C7H10O5/c1-12-7(11)5(8)3-2-4-6(9)10/h2-4H2,1H3,(H,9,10)
**InchiKey:** YPGQZHZBRFDCNW-UHFFFAOYSA-N
**Formula:** C7H10O5
**SMILES:** COC(=O)C(=O)CCCC(=O)O
**Mol. weight [g/mol]:** 174.15

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -620.52 | kJ/mol | Joback Method |
| hf | -810.00 | kJ/mol | Joback Method |
| hfus | 23.96 | kJ/mol | Joback Method |
| hvap | 70.50 | kJ/mol | Joback Method |
| log10ws | 5.56e-03 | | Crippen Method |
| logp | -0.017 | | Crippen Method |
| mcvol | 125.940 | ml/mol | McGowan Method |
| pc | 3782.33 | kPa | Joback Method |
| rinpol | 1281.00 | | NIST Webbook |
| tb | 635.77 | K | Joback Method |
| tc | 821.37 | K | Joback Method |
| tf | 401.49 | K | Joback Method |
| vc | 0.482 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 313.59 | J/mol×K | 635.77 | Joback Method |
| cpg | 321.90 | J/mol×K | 666.70 | Joback Method |
| cpg | 329.79 | J/mol×K | 697.64 | Joback Method |
| cpg | 337.25 | J/mol×K | 728.57 | Joback Method |
| cpg | 344.30 | J/mol×K | 759.50 | Joback Method |
| cpg | 350.92 | J/mol×K | 790.43 | Joback Method |
| cpg | 357.13 | J/mol×K | 821.37 | Joback Method |
| dvisc | 0.0024554 | Pa×s | 401.49 | Joback Method |
| dvisc | 0.0011214 | Pa×s | 440.54 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0005819 | Pa×s | 479.58 | Joback Method |
| dvisc | 0.0003333 | Pa×s | 518.63 | Joback Method |
| dvisc | 0.0002064 | Pa×s | 557.68 | Joback Method |
| dvisc | 0.0001361 | Pa×s | 596.72 | Joback Method |
| dvisc | 0.0000944 | Pa×s | 635.77 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R249197&Units=SI
**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

# 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