# Glutaric acid, di(3-oxobut-2-yl) ester

**Inchi:** InChI=1S/C13H20O6/c1-8(14)10(3)18-12(16)6-5-7-13(17)19-11(4)9(2)15/h10-11H,5-7H2
**InchiKey:** PYEAQKUFCRZTFA-UHFFFAOYSA-N
**Formula:** C13H20O6
**SMILES:** CC(=O)C(C)OC(=O)CCCC(=O)OC(C)C(C)=O
**Mol. weight [g/mol]:** 272.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -671.98 | kJ/mol | Joback Method |
| hf | -1036.97 | kJ/mol | Joback Method |
| hfus | 31.15 | kJ/mol | Joback Method |
| hvap | 75.56 | kJ/mol | Joback Method |
| log10ws | -1.77 | | Crippen Method |
| logp | 1.198 | | Crippen Method |
| mcvol | 212.050 | ml/mol | McGowan Method |
| pc | 2007.30 | kPa | Joback Method |
| rinpol | 1860.00 | | NIST Webbook |
| tb | 756.28 | K | Joback Method |
| tc | 952.49 | K | Joback Method |
| tf | 450.45 | K | Joback Method |
| vc | 0.811 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 607.52 | J/mol×K | 756.28 | Joback Method |
| cpg | 664.21 | J/mol×K | 919.79 | Joback Method |
| cpg | 654.59 | J/mol×K | 887.08 | Joback Method |
| cpg | 644.11 | J/mol×K | 854.38 | Joback Method |
| cpg | 632.77 | J/mol×K | 821.68 | Joback Method |
| cpg | 620.57 | J/mol×K | 788.98 | Joback Method |
| cpg | 672.97 | J/mol×K | 952.49 | Joback Method |
| dvisc | 0.0001103 | Pa×s | 756.28 | Joback Method |
| dvisc | 0.0001447 | Pa×s | 705.31 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001980 | Pa×s | 654.34 | Joback Method |
| dvisc | 0.0002857 | Pa×s | 603.37 | Joback Method |
| dvisc | 0.0004410 | Pa×s | 552.39 | Joback Method |
| dvisc | 0.0007436 | Pa×s | 501.42 | Joback Method |
| dvisc | 0.0014112 | Pa×s | 450.45 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U359715&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

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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 |