# Glutaric acid, 2-methylpent-3-yl isopropyl ester

**Inchi:** InChI=1S/C14H26O4/c1-6-12(10(2)3)18-14(16)9-7-8-13(15)17-11(4)5/h10-12H,6-9H2,1-5

**InchiKey:** IRUFZMHUAVOOCF-UHFFFAOYSA-N

**Formula:** C14H26O4

**SMILES:** CCC(OC(=O)CCCC(=O)OC(C)C)C(C)C

**Mol. weight [g/mol]:** 258.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -408.16 | kJ/mol | Joback Method |
| hf | -837.73 | kJ/mol | Joback Method |
| hfus | 27.02 | kJ/mol | Joback Method |
| hvap | 63.91 | kJ/mol | Joback Method |
| log10ws | -3.39 | | Crippen Method |
| logp | 3.086 | | Crippen Method |
| mcvol | 223.000 | ml/mol | McGowan Method |
| pc | 1671.43 | kPa | Joback Method |
| rinpol | 1556.00 | | NIST Webbook |
| rinpol | 1556.00 | | NIST Webbook |
| tb | 670.98 | K | Joback Method |
| tc | 854.46 | K | Joback Method |
| tf | 346.86 | K | Joback Method |
| vc | 0.850 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 623.56 | J/mol×K | 670.98 | Joback Method |
| cpg | 697.54 | J/mol×K | 823.88 | Joback Method |
| cpg | 684.34 | J/mol×K | 793.30 | Joback Method |
| cpg | 670.35 | J/mol×K | 762.72 | Joback Method |
| cpg | 655.56 | J/mol×K | 732.14 | Joback Method |
| cpg | 639.97 | J/mol×K | 701.56 | Joback Method |
| cpg | 709.94 | J/mol×K | 854.46 | Joback Method |
| dvisc | 0.0000956 | Pa×s | 670.98 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001321 | Pa×s | 616.96 | Joback Method |
| dvisc | 0.0001942 | Pa×s | 562.94 | Joback Method |
| dvisc | 0.0003099 | Pa×s | 508.92 | Joback Method |
| dvisc | 0.0005527 | Pa×s | 454.90 | Joback Method |
| dvisc | 0.0011517 | Pa×s | 400.88 | Joback Method |
| dvisc | 0.0030168 | Pa×s | 346.86 | Joback Method |

# Sources

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|---|---|
| **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=U393370&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |