# Glutaric acid, 3-methylbut-2-en-1-yl 2-methylpentyl ester

**Inchi:** InChI=1S/C16H28O4/c1-5-7-14(4)12-20-16(18)9-6-8-15(17)19-11-10-13(2)3/h10,14H,5-9
**InchiKey:** GVDUHUROBXZEDR-UHFFFAOYSA-N
**Formula:** C16H28O4
**SMILES:** CCCC(C)COC(=O)CCCC(=O)OCC=C(C)C
**Mol. weight [g/mol]:** 284.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -314.77 | kJ/mol | Joback Method |
| hf | -761.02 | kJ/mol | Joback Method |
| hfus | 38.14 | kJ/mol | Joback Method |
| hvap | 69.17 | kJ/mol | Joback Method |
| log10ws | -3.86 | | Crippen Method |
| logp | 3.645 | | Crippen Method |
| mcvol | 246.880 | ml/mol | McGowan Method |
| pc | 1482.71 | kPa | Joback Method |
| rinpol | 1894.00 | | NIST Webbook |
| rinpol | 1894.00 | | NIST Webbook |
| tb | 721.66 | K | Joback Method |
| tc | 906.27 | K | Joback Method |
| tf | 380.36 | K | Joback Method |
| vc | 0.955 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 710.57 | J/mol×K | 721.66 | Joback Method |
| cpg | 726.98 | J/mol×K | 752.43 | Joback Method |
| cpg | 742.54 | J/mol×K | 783.20 | Joback Method |
| cpg | 757.26 | J/mol×K | 813.96 | Joback Method |
| cpg | 771.17 | J/mol×K | 844.73 | Joback Method |
| cpg | 784.28 | J/mol×K | 875.50 | Joback Method |
| cpg | 796.60 | J/mol×K | 906.27 | Joback Method |

# Sources

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|---|---|
| **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=U391706&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |