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

**Inchi:** InChI=1S/C15H26O4/c1-12(2)9-10-18-13(16)7-6-8-14(17)19-11-15(3,4)5/h9H,6-8,10-11H

**InchiKey:** AETOZYXYJQINMH-UHFFFAOYSA-N

**Formula:** C15H26O4

**SMILES:** CC(C)=CCOC(=O)CCCC(=O)OCC(C)(C)C

**Mol. weight [g/mol]:** 270.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -317.91 | kJ/mol | Joback Method |
| hf | -743.85 | kJ/mol | Joback Method |
| hfus | 31.66 | kJ/mol | Joback Method |
| hvap | 66.04 | kJ/mol | Joback Method |
| log10ws | -3.44 | | Crippen Method |
| logp | 3.255 | | Crippen Method |
| mcvol | 232.790 | ml/mol | McGowan Method |
| pc | 1612.88 | kPa | Joback Method |
| rinpol | 1751.00 | | NIST Webbook |
| rinpol | 1751.00 | | NIST Webbook |
| tb | 695.99 | K | Joback Method |
| tc | 885.91 | K | Joback Method |
| tf | 386.51 | K | Joback Method |
| vc | 0.893 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 656.75 | J/mol×K | 695.99 | Joback Method |
| cpg | 672.92 | J/mol×K | 727.64 | Joback Method |
| cpg | 688.21 | J/mol×K | 759.30 | Joback Method |
| cpg | 702.65 | J/mol×K | 790.95 | Joback Method |
| cpg | 716.27 | J/mol×K | 822.61 | Joback Method |
| cpg | 729.10 | J/mol×K | 854.26 | Joback Method |
| cpg | 741.17 | J/mol×K | 885.91 | 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=U391609&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 |
| **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 |