# Glutaric acid, 3-methylbut-2-en-1-yl 4-nitrophenyl ester

**Inchi:** InChI=1S/C16H19NO6/c1-12(2)10-11-22-15(18)4-3-5-16(19)23-14-8-6-13(7-9-14)17(20)
**InchiKey:** MJCSEGGICGOWBD-UHFFFAOYSA-N
**Formula:** C16H19NO6
**SMILES:** CC(C)=CCOC(=O)CCCC(=O)Oc1ccc([N+](=O)[O-])cc1
**Mol. weight [g/mol]:** 321.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -174.00 | kJ/mol | Joback Method |
| hf | -541.44 | kJ/mol | Joback Method |
| hfus | 46.67 | kJ/mol | Joback Method |
| hvap | 89.09 | kJ/mol | Joback Method |
| log10ws | -4.50 | | Crippen Method |
| logp | 3.180 | | Crippen Method |
| mcvol | 240.540 | ml/mol | McGowan Method |
| pc | 1928.74 | kPa | Joback Method |
| rinpol | 2505.00 | | NIST Webbook |
| rinpol | 2505.00 | | NIST Webbook |
| tb | 905.60 | K | Joback Method |
| tc | 1135.73 | K | Joback Method |
| tf | 577.91 | K | Joback Method |
| vc | 0.934 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 726.42 | J/mol×K | 905.60 | Joback Method |
| cpg | 738.27 | J/mol×K | 943.95 | Joback Method |
| cpg | 749.03 | J/mol×K | 982.31 | Joback Method |
| cpg | 758.73 | J/mol×K | 1020.66 | Joback Method |
| cpg | 767.42 | J/mol×K | 1059.02 | Joback Method |
| cpg | 775.13 | J/mol×K | 1097.37 | Joback Method |
| cpg | 781.91 | J/mol×K | 1135.73 | 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=U391972&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 |