# Glutaric acid, di(4-nitrophenyl) ester

**Inchi:** InChI=1S/C17H14N2O8/c20-16(26-14-8-4-12(5-9-14)18(22)23)2-1-3-17(21)27-15-10-6-1
**InchiKey:** IOIJXIHQQRSQDS-UHFFFAOYSA-N
**Formula:** C17H14N2O8
**SMILES:** O=C(CCCC(=O)Oc1ccc([N+](=O)[O-])cc1)Oc1ccc([N+](=O)[O-])cc1
**Mol. weight [g/mol]:** 374.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -98.92 | kJ/mol | Joback Method |
| hf | -455.21 | kJ/mol | Joback Method |
| hfus | 55.39 | kJ/mol | Joback Method |
| hvap | 110.81 | kJ/mol | Joback Method |
| log10ws | -5.47 | | Crippen Method |
| logp | 3.184 | | Crippen Method |
| mcvol | 252.590 | ml/mol | McGowan Method |
| pc | 2263.26 | kPa | Joback Method |
| rinpol | 3316.00 | | NIST Webbook |
| rinpol | 3316.00 | | NIST Webbook |
| tb | 1107.94 | K | Joback Method |
| tc | 1375.35 | K | Joback Method |
| tf | 790.77 | K | Joback Method |
| vc | 0.984 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 779.53 | J/mol×K | 1107.94 | Joback Method |
| cpg | 784.66 | J/mol×K | 1152.51 | Joback Method |
| cpg | 788.33 | J/mol×K | 1197.08 | Joback Method |
| cpg | 790.60 | J/mol×K | 1241.64 | Joback Method |
| cpg | 791.53 | J/mol×K | 1286.21 | Joback Method |
| cpg | 791.17 | J/mol×K | 1330.78 | Joback Method |
| cpg | 789.57 | J/mol×K | 1375.35 | 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=U391981&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 |
| **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 |