# Glutaric acid, 2-nitro-4-chlorobenzyl undecyl ester

**Inchi:** InChI=1S/C23H34ClNO6/c1-2-3-4-5-6-7-8-9-10-16-30-22(26)12-11-13-23(27)31-18-19-1

**InchiKey:** JULZITCBXSKIJB-UHFFFAOYSA-N

**Formula:** C23H34ClNO6

**SMILES:** CCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(Cl)cc1[N+](=O)[O-]

**Mol. weight [g/mol]:** 455.97

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -208.29 | kJ/mol | Joback Method |
| hf | -820.56 | kJ/mol | Joback Method |
| hfus | 69.72 | kJ/mol | Joback Method |
| hvap | 109.68 | kJ/mol | Joback Method |
| log10ws | -8.11 | | Crippen Method |
| logp | 6.536 | | Crippen Method |
| mcvol | 355.710 | ml/mol | McGowan Method |
| pc | 1069.36 | kPa | Joback Method |
| rinpol | 3293.00 | | NIST Webbook |
| tb | 1104.13 | K | Joback Method |
| tc | 1353.02 | K | Joback Method |
| tf | 718.28 | K | Joback Method |
| vc | 1.395 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1187.24 | J/mol×K | 1104.13 | Joback Method |
| cpg | 1198.65 | J/mol×K | 1145.61 | Joback Method |
| cpg | 1208.39 | J/mol×K | 1187.09 | Joback Method |
| cpg | 1216.52 | J/mol×K | 1228.57 | Joback Method |
| cpg | 1223.10 | J/mol×K | 1270.06 | Joback Method |
| cpg | 1228.19 | J/mol×K | 1311.54 | Joback Method |
| cpg | 1231.85 | J/mol×K | 1353.02 | 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=U377056&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 |