# Glutaric acid, heptyl 2-nitro-3-chlorobenzyl ester

**Inchi:** InChI=1S/C19H26ClNO6/c1-2-3-4-5-6-13-26-17(22)11-8-12-18(23)27-14-15-9-7-10-16(2

**InchiKey:** NIFPTEIDFXIQCW-UHFFFAOYSA-N

**Formula:** C19H26ClNO6

**SMILES:** CCCCCCCOC(=O)CCCC(=O)OCc1cccc(Cl)c1[N+](=O)[O-]

**Mol. weight [g/mol]:** 399.87

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -241.97 | kJ/mol | Joback Method |
| hf | -738.00 | kJ/mol | Joback Method |
| hfus | 59.36 | kJ/mol | Joback Method |
| hvap | 100.78 | kJ/mol | Joback Method |
| log10ws | -6.43 | | Crippen Method |
| logp | 4.975 | | Crippen Method |
| mcvol | 299.350 | ml/mol | McGowan Method |
| pc | 1398.55 | kPa | Joback Method |
| rinpol | 2875.00 | | NIST Webbook |
| rinpol | 2875.00 | | NIST Webbook |
| tb | 1012.61 | K | Joback Method |
| tc | 1243.24 | K | Joback Method |
| tf | 673.20 | K | Joback Method |
| vc | 1.171 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 948.42 | J/mol×K | 1012.61 | Joback Method |
| cpg | 959.47 | J/mol×K | 1051.05 | Joback Method |
| cpg | 969.17 | J/mol×K | 1089.49 | Joback Method |
| cpg | 977.55 | J/mol×K | 1127.93 | Joback Method |
| cpg | 984.64 | J/mol×K | 1166.36 | Joback Method |
| cpg | 990.48 | J/mol×K | 1204.80 | Joback Method |
| cpg | 995.09 | J/mol×K | 1243.24 | 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=U377030&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 |