# Glutaric acid, 2-methylhex-3-yl 3-nitrobenzyl ester

**Inchi:** InChI=1S/C19H27NO6/c1-4-7-17(14(2)3)26-19(22)11-6-10-18(21)25-13-15-8-5-9-16(12-
**InchiKey:** RVVZWLXMRHQYTK-UHFFFAOYSA-N
**Formula:** C19H27NO6
**SMILES:** CCCC(OC(=O)CCCC(=O)OCc1cccc([N+](=O)[O-])c1)C(C)C
**Mol. weight [g/mol]:** 365.42

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -225.29 | kJ/mol | Joback Method |
| hf | -721.35 | kJ/mol | Joback Method |
| hfus | 48.51 | kJ/mol | Joback Method |
| hvap | 94.95 | kJ/mol | Joback Method |
| log10ws | -5.62 | | Crippen Method |
| logp | 4.176 | | Crippen Method |
| mcvol | 287.110 | ml/mol | McGowan Method |
| pc | 1472.49 | kPa | Joback Method |
| rinpol | 2757.00 | | NIST Webbook |
| tb | 969.32 | K | Joback Method |
| tc | 1195.93 | K | Joback Method |
| tf | 600.76 | K | Joback Method |
| vc | 1.109 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 930.05 | J/mol×K | 969.32 | Joback Method |
| cpg | 942.58 | J/mol×K | 1007.09 | Joback Method |
| cpg | 953.75 | J/mol×K | 1044.86 | Joback Method |
| cpg | 963.59 | J/mol×K | 1082.62 | Joback Method |
| cpg | 972.14 | J/mol×K | 1120.39 | Joback Method |
| cpg | 979.43 | J/mol×K | 1158.16 | Joback Method |
| cpg | 985.50 | J/mol×K | 1195.93 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U377463&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |