# Glutaric acid, butyl 3-methyl-2-nitrobenzyl ester

**Inchi:** InChI=1S/C17H23NO6/c1-3-4-11-23-15(19)9-6-10-16(20)24-12-14-8-5-7-13(2)17(14)18(

**InchiKey:** YUVWWAMNFRUVSZ-UHFFFAOYSA-N

**Formula:** C17H23NO6

**SMILES:** CCCCOC(=O)CCCC(=O)OCc1cccc(C)c1[N+](=O)[O-]

**Mol. weight [g/mol]:** 337.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -246.88 | kJ/mol | Joback Method |
| hf | -680.98 | kJ/mol | Joback Method |
| hfus | 49.98 | kJ/mol | Joback Method |
| hvap | 91.94 | kJ/mol | Joback Method |
| log10ws | -4.97 | | Crippen Method |
| logp | 3.460 | | Crippen Method |
| mcvol | 258.930 | ml/mol | McGowan Method |
| pc | 1672.79 | kPa | Joback Method |
| rinpol | 2470.00 | | NIST Webbook |
| rinpol | 2470.00 | | NIST Webbook |
| tb | 929.42 | K | Joback Method |
| tc | 1152.32 | K | Joback Method |
| tf | 620.74 | K | Joback Method |
| vc | 1.010 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 811.03 | J/mol×K | 929.42 | Joback Method |
| cpg | 823.17 | J/mol×K | 966.57 | Joback Method |
| cpg | 834.07 | J/mol×K | 1003.72 | Joback Method |
| cpg | 843.77 | J/mol×K | 1040.87 | Joback Method |
| cpg | 852.26 | J/mol×K | 1078.02 | Joback Method |
| cpg | 859.58 | J/mol×K | 1115.17 | Joback Method |
| cpg | 865.74 | J/mol×K | 1152.32 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U376733&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

| | |
|---|---|
| **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 |

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