# Glutaric acid, 3-methoxy-4-nitrobenzyl butyl ester

**Inchi:** InChI=1S/C17H23NO7/c1-3-4-10-24-16(19)6-5-7-17(20)25-12-13-8-9-14(18(21)22)15(11

**InchiKey:** FWBPSEZUORPULU-UHFFFAOYSA-N

**Formula:** C17H23NO7

**SMILES:** CCCCOC(=O)CCCC(=O)OCc1ccc([N+](=O)[O-])c(OC)c1

**Mol. weight [g/mol]:** 353.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -351.88 | kJ/mol | Joback Method |
| hf | -813.20 | kJ/mol | Joback Method |
| hfus | 51.17 | kJ/mol | Joback Method |
| hvap | 94.35 | kJ/mol | Joback Method |
| log10ws | -4.61 | | Crippen Method |
| logp | 3.160 | | Crippen Method |
| mcvol | 264.800 | ml/mol | McGowan Method |
| pc | 1649.77 | kPa | Joback Method |
| rinpol | 2750.00 | | NIST Webbook |
| rinpol | 2750.00 | | NIST Webbook |
| tb | 951.84 | K | Joback Method |
| tc | 1175.57 | K | Joback Method |
| tf | 642.97 | K | Joback Method |
| vc | 1.028 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 837.16 | J/mol×K | 951.84 | Joback Method |
| cpg | 848.49 | J/mol×K | 989.13 | Joback Method |
| cpg | 858.45 | J/mol×K | 1026.42 | Joback Method |
| cpg | 867.04 | J/mol×K | 1063.71 | Joback Method |
| cpg | 874.26 | J/mol×K | 1100.99 | Joback Method |
| cpg | 880.11 | J/mol×K | 1138.28 | Joback Method |
| cpg | 884.59 | J/mol×K | 1175.57 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U376891&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 |