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

**Inchi:** InChI=1S/C25H39NO6/c1-3-4-5-6-7-8-9-10-11-12-19-31-23(27)17-14-18-24(28)32-20-22

**InchiKey:** OTYIZIIDOXBMPB-UHFFFAOYSA-N

**Formula:** C25H39NO6

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

**Mol. weight [g/mol]:** 449.58

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -179.52 | kJ/mol | Joback Method |
| hf | -846.10 | kJ/mol | Joback Method |
| hfus | 70.70 | kJ/mol | Joback Method |
| hvap | 109.75 | kJ/mol | Joback Method |
| log10ws | -8.32 | | Crippen Method |
| logp | 6.581 | | Crippen Method |
| mcvol | 371.650 | ml/mol | McGowan Method |
| pc | 968.68 | kPa | Joback Method |
| rinpol | 3301.00 | | NIST Webbook |
| rinpol | 3301.00 | | NIST Webbook |
| tb | 1112.46 | K | Joback Method |
| tc | 1366.14 | K | Joback Method |
| tf | 710.90 | K | Joback Method |
| vc | 1.458 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1289.76 | J/mol×K | 1112.46 | Joback Method |
| cpg | 1302.71 | J/mol×K | 1154.74 | Joback Method |
| cpg | 1313.81 | J/mol×K | 1197.02 | Joback Method |
| cpg | 1323.12 | J/mol×K | 1239.30 | Joback Method |
| cpg | 1330.72 | J/mol×K | 1281.58 | Joback Method |
| cpg | 1336.68 | J/mol×K | 1323.86 | Joback Method |
| cpg | 1341.06 | J/mol×K | 1366.14 | Joback Method |

# Sources

| | |
|---|---|
| **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=U376742&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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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