# Glutaric acid, monoamide, N-(3-pentyl)-, butyl ester

**Inchi:** InChI=1S/C14H27NO3/c1-4-7-11-18-14(17)10-8-9-13(16)15-12(5-2)6-3/h12H,4-11H2,1-3

**InchiKey:** RMHYACMHJPHUDN-UHFFFAOYSA-N

**Formula:** C14H27NO3

**SMILES:** CCCCOC(=O)CCCC(=O)NC(CC)CC

**Mol. weight [g/mol]:** 257.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -208.89 | kJ/mol | Joback Method |
| hf | -641.48 | kJ/mol | Joback Method |
| hfus | 37.98 | kJ/mol | Joback Method |
| hvap | 68.71 | kJ/mol | Joback Method |
| log10ws | -3.62 | | Crippen Method |
| logp | 2.805 | | Crippen Method |
| mcvol | 227.110 | ml/mol | McGowan Method |
| pc | 1690.72 | kPa | Joback Method |
| rinpol | 1913.00 | | NIST Webbook |
| tb | 699.61 | K | Joback Method |
| tc | 880.88 | K | Joback Method |
| tf | 407.29 | K | Joback Method |
| vc | 0.878 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 652.56 | J/mol×K | 699.61 | Joback Method |
| cpg | 668.33 | J/mol×K | 729.82 | Joback Method |
| cpg | 683.30 | J/mol×K | 760.03 | Joback Method |
| cpg | 697.48 | J/mol×K | 790.25 | Joback Method |
| cpg | 710.90 | J/mol×K | 820.46 | Joback Method |
| cpg | 723.56 | J/mol×K | 850.67 | Joback Method |
| cpg | 735.48 | J/mol×K | 880.88 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U360809&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 |