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

**Inchi:** InChI=1S/C16H31NO3/c1-4-7-8-9-13-20-16(19)12-10-11-15(18)17-14(5-2)6-3/h14H,4-13

**InchiKey:** PYLNDCYJIDNGMA-UHFFFAOYSA-N

**Formula:** C16H31NO3

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

**Mol. weight [g/mol]:** 285.42

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -192.05 | kJ/mol | Joback Method |
| hf | -682.76 | kJ/mol | Joback Method |
| hfus | 43.16 | kJ/mol | Joback Method |
| hvap | 73.16 | kJ/mol | Joback Method |
| log10ws | -4.46 | | Crippen Method |
| logp | 3.585 | | Crippen Method |
| mcvol | 255.290 | ml/mol | McGowan Method |
| pc | 1452.35 | kPa | Joback Method |
| rinpol | 2109.00 | | NIST Webbook |
| tb | 745.37 | K | Joback Method |
| tc | 926.90 | K | Joback Method |
| tf | 429.83 | K | Joback Method |
| vc | 0.991 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 765.34 | J/mol×K | 745.37 | Joback Method |
| cpg | 781.92 | J/mol×K | 775.63 | Joback Method |
| cpg | 797.62 | J/mol×K | 805.88 | Joback Method |
| cpg | 812.46 | J/mol×K | 836.14 | Joback Method |
| cpg | 826.46 | J/mol×K | 866.39 | Joback Method |
| cpg | 839.64 | J/mol×K | 896.65 | Joback Method |
| cpg | 852.02 | J/mol×K | 926.90 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U360811&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 |