# Glutaric acid, monoamide, N-(1-phenylethyl)-, pentadecyl ester

**Inchi:** InChI=1S/C28H47NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-18-24-32-28(31)23-19-22-27(30
**InchiKey:** NEGHMFFEXFRSGF-UHFFFAOYSA-N
**Formula:** C28H47NO3
**SMILES:** CCCCCCCCCCCCCCCOC(=O)CCCC(=O)NC(C)c1ccccc1
**Mol. weight [g/mol]:** 445.68

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 21.40 | kJ/mol | Joback Method |
| hf | -693.91 | kJ/mol | Joback Method |
| hfus | 68.28 | kJ/mol | Joback Method |
| hvap | 102.15 | kJ/mol | Joback Method |
| log10ws | -8.93 | | Crippen Method |
| logp | 7.668 | | Crippen Method |
| mcvol | 400.610 | ml/mol | McGowan Method |
| pc | 842.60 | kPa | Joback Method |
| rinpol | 3445.00 | | NIST Webbook |
| rinpol | 3445.00 | | NIST Webbook |
| tb | 1046.61 | K | Joback Method |
| tc | 1287.21 | K | Joback Method |
| tf | 591.49 | K | Joback Method |
| vc | 1.554 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1402.96 | J/mol×K | 1046.61 | Joback Method |
| cpg | 1421.42 | J/mol×K | 1086.71 | Joback Method |
| cpg | 1438.25 | J/mol×K | 1126.81 | Joback Method |
| cpg | 1453.56 | J/mol×K | 1166.91 | Joback Method |
| cpg | 1467.46 | J/mol×K | 1207.01 | Joback Method |
| cpg | 1480.07 | J/mol×K | 1247.11 | Joback Method |
| cpg | 1491.49 | J/mol×K | 1287.21 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U360164&Units=SI |

# 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 |