# Glutaric acid, monoamide, N-(2-octyl)-, ethyl ester

**Inchi:** InChI=1S/C15H29NO3/c1-4-6-7-8-10-13(3)16-14(17)11-9-12-15(18)19-5-2/h13H,4-12H2

**InchiKey:** ZJOCAIIOFNYCOY-UHFFFAOYSA-N

**Formula:** C15H29NO3

**SMILES:** CCCCCCC(C)NC(=O)CCCC(=O)OCC

**Mol. weight [g/mol]:** 271.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -200.47 | kJ/mol | Joback Method |
| hf | -662.12 | kJ/mol | Joback Method |
| hfus | 40.57 | kJ/mol | Joback Method |
| hvap | 70.93 | kJ/mol | Joback Method |
| log10ws | -4.04 | | Crippen Method |
| logp | 3.195 | | Crippen Method |
| mcvol | 241.200 | ml/mol | McGowan Method |
| pc | 1564.75 | kPa | Joback Method |
| rinpol | 2344.00 | | NIST Webbook |
| tb | 722.49 | K | Joback Method |
| tc | 903.63 | K | Joback Method |
| tf | 418.56 | K | Joback Method |
| vc | 0.934 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 708.39 | J/mol×K | 722.49 | Joback Method |
| cpg | 724.58 | J/mol×K | 752.68 | Joback Method |
| cpg | 739.93 | J/mol×K | 782.87 | Joback Method |
| cpg | 754.45 | J/mol×K | 813.06 | Joback Method |
| cpg | 768.17 | J/mol×K | 843.25 | Joback Method |
| cpg | 781.11 | J/mol×K | 873.44 | Joback Method |
| cpg | 793.27 | J/mol×K | 903.63 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U360850&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 |

# 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 |