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

**Inchi:** InChI=1S/C17H33NO3/c1-4-6-8-9-11-15(3)18-16(19)12-10-13-17(20)21-14-7-5-2/h15H,4

**InchiKey:** CQNKRSFCJKACCX-UHFFFAOYSA-N

**Formula:** C17H33NO3

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

**Mol. weight [g/mol]:** 299.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -183.63 | kJ/mol | Joback Method |
| hf | -703.40 | kJ/mol | Joback Method |
| hfus | 45.75 | kJ/mol | Joback Method |
| hvap | 75.39 | kJ/mol | Joback Method |
| log10ws | -4.88 | | Crippen Method |
| logp | 3.975 | | Crippen Method |
| mcvol | 269.380 | ml/mol | McGowan Method |
| pc | 1351.64 | kPa | Joback Method |
| rinpol | 2550.00 | | NIST Webbook |
| tb | 768.25 | K | Joback Method |
| tc | 950.75 | K | Joback Method |
| tf | 441.10 | K | Joback Method |
| vc | 1.046 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 823.32 | J/mol×K | 768.25 | Joback Method |
| cpg | 840.28 | J/mol×K | 798.67 | Joback Method |
| cpg | 856.32 | J/mol×K | 829.08 | Joback Method |
| cpg | 871.45 | J/mol×K | 859.50 | Joback Method |
| cpg | 885.72 | J/mol×K | 889.92 | Joback Method |
| cpg | 899.12 | J/mol×K | 920.33 | Joback Method |
| cpg | 911.70 | J/mol×K | 950.75 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U360853&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

| | |
|---|---|
| **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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