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

**Inchi:** InChI=1S/C22H35NO3/c1-3-4-5-6-7-11-17-26-22(25)16-12-15-21(24)23-18-19(2)20-13-9

**InchiKey:** JLDMJXIZGOTSRQ-UHFFFAOYSA-N

**Formula:** C22H35NO3

**SMILES:** CCCCCCCCOC(=O)CCCC(=O)NCC(C)c1ccccc1

**Mol. weight [g/mol]:** 361.52

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -29.12 | kJ/mol | Joback Method |
| hf | -570.07 | kJ/mol | Joback Method |
| hfus | 52.74 | kJ/mol | Joback Method |
| hvap | 88.79 | kJ/mol | Joback Method |
| log10ws | -5.93 | | Crippen Method |
| logp | 4.980 | | Crippen Method |
| mcvol | 316.070 | ml/mol | McGowan Method |
| pc | 1214.90 | kPa | Joback Method |
| rinpol | 2824.00 | | NIST Webbook |
| tb | 909.33 | K | Joback Method |
| tc | 1117.03 | K | Joback Method |
| tf | 523.87 | K | Joback Method |
| vc | 1.218 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1029.29 | J/mol×K | 909.33 | Joback Method |
| cpg | 1045.71 | J/mol×K | 943.95 | Joback Method |
| cpg | 1060.93 | J/mol×K | 978.56 | Joback Method |
| cpg | 1074.99 | J/mol×K | 1013.18 | Joback Method |
| cpg | 1087.95 | J/mol×K | 1047.80 | Joback Method |
| cpg | 1099.87 | J/mol×K | 1082.41 | Joback Method |
| cpg | 1110.79 | J/mol×K | 1117.03 | 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=U360826&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 |