# Glutaric acid, monoamide, N-(4-chlorophenyl)-, undecyl ester

**Inchi:** InChI=1S/C22H34ClNO3/c1-2-3-4-5-6-7-8-9-10-18-27-22(26)13-11-12-21(25)24-20-16-1

**InchiKey:** BOICXXMTAGMLRZ-UHFFFAOYSA-N

**Formula:** C22H34ClNO3

**SMILES:** CCCCCCCCCCCOC(=O)CCCC(=O)Nc1ccc(Cl)cc1

**Mol. weight [g/mol]:** 395.96

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -48.24 | kJ/mol | Joback Method |
| hf | -592.00 | kJ/mol | Joback Method |
| hfus | 60.07 | kJ/mol | Joback Method |
| hvap | 94.23 | kJ/mol | Joback Method |
| log10ws | -7.08 | | Crippen Method |
| logp | 6.523 | | Crippen Method |
| mcvol | 328.310 | ml/mol | McGowan Method |
| pc | 1165.63 | kPa | Joback Method |
| rinpol | 3354.00 | | NIST Webbook |
| rinpol | 3354.00 | | NIST Webbook |
| tb | 952.18 | K | Joback Method |
| tc | 1166.90 | K | Joback Method |
| tf | 581.31 | K | Joback Method |
| vc | 1.274 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1054.39 | J/mol×K | 952.18 | Joback Method |
| cpg | 1069.62 | J/mol×K | 987.97 | Joback Method |
| cpg | 1083.64 | J/mol×K | 1023.75 | Joback Method |
| cpg | 1096.50 | J/mol×K | 1059.54 | Joback Method |
| cpg | 1108.27 | J/mol×K | 1095.32 | Joback Method |
| cpg | 1119.00 | J/mol×K | 1131.11 | Joback Method |
| cpg | 1128.73 | J/mol×K | 1166.90 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U360790&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

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