

# Glutaric acid, monoamide, N-(2-methoxyphenyl)-, decyl ester

**Inchi:** InChI=1S/C22H35NO4/c1-3-4-5-6-7-8-9-12-18-27-22(25)17-13-16-21(24)23-19-14-10-11  
**InchiKey:** ZQWUDGMMDNUMSI-UHFFFAOYSA-N  
**Formula:** C22H35NO4  
**SMILES:** CCCCCCCCCCOC(=O)CCCC(=O)Nc1ccccc1OC  
**Mol. weight [g/mol]:** 377.52

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -141.31 | kJ/mol  | Joback Method  |
| hf            | -708.48 | kJ/mol  | Joback Method  |
| hfus          | 57.06   | kJ/mol  | Joback Method  |
| hvap          | 92.25   | kJ/mol  | Joback Method  |
| log10ws       | -6.10   |         | Crippen Method |
| logp          | 5.488   |         | Crippen Method |
| mcvol         | 321.940 | ml/mol  | McGowan Method |
| pc            | 1181.71 | kPa     | Joback Method  |
| rinpol        | 3266.00 |         | NIST Webbook   |
| rinpol        | 3266.00 |         | NIST Webbook   |
| tb            | 937.17  | K       | Joback Method  |
| tc            | 1148.38 | K       | Joback Method  |
| tf            | 573.62  | K       | Joback Method  |
| vc            | 1.242   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1057.55 | J/mol×K | 937.17          | Joback Method |
| cpg           | 1073.28 | J/mol×K | 972.37          | Joback Method |
| cpg           | 1087.68 | J/mol×K | 1007.57         | Joback Method |
| cpg           | 1100.79 | J/mol×K | 1042.78         | Joback Method |
| cpg           | 1112.65 | J/mol×K | 1077.98         | Joback Method |
| cpg           | 1123.28 | J/mol×K | 1113.18         | Joback Method |
| cpg           | 1132.73 | J/mol×K | 1148.38         | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U360937&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360937&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpola:</b> | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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