

# Glutaric acid, monoamide, N-dodecyl-, propyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C20H39NO3/c1-3-5-6-7-8-9-10-11-12-13-17-21-19(22)15-14-16-20(23)24-18-4 |
| InchiKey:            | AKTYSPUWGSROMT-UHFFFAOYSA-N  |
| Formula:             | C20H39NO3  |
| SMILES:              | CCCCCCCCCCCCNC(=O)CCCC(=O)OCCC   |
| Mol. weight [g/mol]: | 341.53   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -155.93 | kJ/mol               | Joback Method  |
| hf            | -760.04 | kJ/mol               | Joback Method  |
| hfus          | 57.04   | kJ/mol               | Joback Method  |
| hvap          | 82.45   | kJ/mol               | Joback Method  |
| log10ws       | -6.02   |                      | Crippen Method |
| logp          | 5.147   |                      | Crippen Method |
| mvol          | 311.650 | ml/mol               | McGowan Method |
| pc            | 1099.35 | kPa                  | Joback Method  |
| rinpol        | 3026.00 |                      | NIST Webbook   |
| rinpol        | 3026.00 |                      | NIST Webbook   |
| tb            | 837.33  | K                    | Joback Method  |
| tc            | 1026.23 | K                    | Joback Method  |
| tf            | 489.91  | K                    | Joback Method  |
| vc            | 1.220   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1002.22 | J/mol×K | 837.33          | Joback Method |
| cpg           | 1020.30 | J/mol×K | 868.81          | Joback Method |
| cpg           | 1037.33 | J/mol×K | 900.30          | Joback Method |
| cpg           | 1053.32 | J/mol×K | 931.78          | Joback Method |
| cpg           | 1068.31 | J/mol×K | 963.26          | Joback Method |
| cpg           | 1082.33 | J/mol×K | 994.74          | Joback Method |
| cpg           | 1095.41 | J/mol×K | 1026.23         | 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=U360866&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360866&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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