

# Glutaric acid, 2-propylpentyl undecyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C24H46O4/c1-4-7-8-9-10-11-12-13-14-20-27-23(25)18-15-19-24(26)28-21-22( |
| <b>InchiKey:</b>            | SUDKIPDFEBCBHQ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C24H46O4   |
| <b>SMILES:</b>              | CCCCCCCCCOC(=O)CCCC(=O)OCC(CCC)CCC   |
| <b>Mol. weight [g/mol]:</b> | 398.62   |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -319.08  | kJ/mol               | Joback Method  |
| hf            | -1033.57 | kJ/mol               | Joback Method  |
| hfus          | 59.97    | kJ/mol               | Joback Method  |
| hvap          | 86.94    | kJ/mol               | Joback Method  |
| log10ws       | -7.35    |                      | Crippen Method |
| logp          | 6.990    |                      | Crippen Method |
| mvol          | 363.900  | ml/mol               | McGowan Method |
| pc            | 853.96   | kPa                  | Joback Method  |
| rinpol        | 2713.00  |                      | NIST Webbook   |
| rinpol        | 2713.00  |                      | NIST Webbook   |
| tb            | 900.66   | K                    | Joback Method  |
| tc            | 1103.57  | K                    | Joback Method  |
| tf            | 489.56   | K                    | Joback Method  |
| vc            | 1.421    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1218.00   | J/molxK | 900.66          | Joback Method |
| cpg           | 1238.11   | J/molxK | 934.48          | Joback Method |
| cpg           | 1256.81   | J/molxK | 968.30          | Joback Method |
| cpg           | 1274.13   | J/molxK | 1002.12         | Joback Method |
| cpg           | 1290.12   | J/molxK | 1035.94         | Joback Method |
| cpg           | 1304.80   | J/molxK | 1069.75         | Joback Method |
| cpg           | 1318.20   | J/molxK | 1103.57         | Joback Method |
| dvisc         | 0.0006076 | Paxs    | 489.56          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002626 | Paxs | 558.08 | Joback Method |
| dvisc | 0.0001364 | Paxs | 626.59 | Joback Method |
| dvisc | 0.0000806 | Paxs | 695.11 | Joback Method |
| dvisc | 0.0000523 | Paxs | 763.63 | Joback Method |
| dvisc | 0.0000365 | Paxs | 832.14 | Joback Method |
| dvisc | 0.0000269 | Paxs | 900.66 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <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=U377140&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377140&amp;Units=SI</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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>rinpol:</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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