

# Glutaric acid, dec-2-yl 2-octyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C23H44O4/c1-5-7-9-11-12-14-17-21(4)27-23(25)19-15-18-22(24)26-20(3)16-1 |
| <b>InchiKey:</b>            | FTVZPPQJIHHVDL-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C23H44O4   |
| <b>SMILES:</b>              | CCCCCCCCC(C)OC(=O)CCCC(=O)OC(C)CCCCC   |
| <b>Mol. weight [g/mol]:</b> | 384.59   |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -329.94  | kJ/mol               | Joback Method  |
| hf            | -1018.21 | kJ/mol               | Joback Method  |
| hfus          | 53.85    | kJ/mol               | Joback Method  |
| hvap          | 84.33    | kJ/mol               | Joback Method  |
| log10ws       | -7.40    |                      | Crippen Method |
| logp          | 6.741    |                      | Crippen Method |
| mvol          | 349.810  | ml/mol               | McGowan Method |
| pc            | 908.34   | kPa                  | Joback Method  |
| rinpol        | 2457.00  |                      | NIST Webbook   |
| rinpol        | 2457.00  |                      | NIST Webbook   |
| tb            | 877.34   | K                    | Joback Method  |
| tc            | 1074.11  | K                    | Joback Method  |
| tf            | 463.29   | K                    | Joback Method  |
| vc            | 1.359    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1155.40   | J/molxK | 877.34          | Joback Method |
| cpg           | 1240.52   | J/molxK | 1041.32         | Joback Method |
| cpg           | 1226.01   | J/molxK | 1008.52         | Joback Method |
| cpg           | 1210.26   | J/molxK | 975.73          | Joback Method |
| cpg           | 1193.27   | J/molxK | 942.93          | Joback Method |
| cpg           | 1174.99   | J/molxK | 910.14          | Joback Method |
| cpg           | 1253.84   | J/molxK | 1074.11         | Joback Method |
| dvisc         | 0.0000286 | Paxs    | 877.34          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000394 | Paxs | 808.33 | Joback Method |
| dvisc | 0.0000577 | Paxs | 739.32 | Joback Method |
| dvisc | 0.0000911 | Paxs | 670.32 | Joback Method |
| dvisc | 0.0001600 | Paxs | 601.31 | Joback Method |
| dvisc | 0.0003252 | Paxs | 532.30 | Joback Method |
| dvisc | 0.0008160 | Paxs | 463.29 | 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=U391454&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391454&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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