

# Glutaric acid, hex-2-en-1-yl dec-2-yl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C21H38O4/c1-4-6-8-10-11-12-15-19(3)25-21(23)17-14-16-20(22)24-18-13-9-7 |
| <b>InchiKey:</b>            | BXAZWKIPTUHQFT-UKTHLTGXSA-N  |
| <b>Formula:</b>             | C21H38O4   |
| <b>SMILES:</b>              | CCCC=CCOC(=O)CCCC(=O)OC(C)CCCCCCCC   |
| <b>Mol. weight [g/mol]:</b> | 354.52   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -264.12 | kJ/mol               | Joback Method  |
| hf            | -854.43 | kJ/mol               | Joback Method  |
| hfus          | 52.40   | kJ/mol               | Joback Method  |
| hvap          | 80.22   | kJ/mol               | Joback Method  |
| log10ws       | -6.30   |                      | Crippen Method |
| logp          | 5.739   |                      | Crippen Method |
| mcvol         | 317.330 | ml/mol               | McGowan Method |
| pc            | 1052.77 | kPa                  | Joback Method  |
| rinpola       | 2318.00 |                      | NIST Webbook   |
| tb            | 836.18  | K                    | Joback Method  |
| tc            | 1026.01 | K                    | Joback Method  |
| tf            | 450.67  | K                    | Joback Method  |
| vc            | 1.234   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1004.95   | J/molxK | 836.18          | Joback Method |
| cpg           | 1023.11   | J/molxK | 867.82          | Joback Method |
| cpg           | 1040.19   | J/molxK | 899.46          | Joback Method |
| cpg           | 1056.24   | J/molxK | 931.09          | Joback Method |
| cpg           | 1071.28   | J/molxK | 962.73          | Joback Method |
| cpg           | 1085.33   | J/molxK | 994.37          | Joback Method |
| cpg           | 1098.44   | J/molxK | 1026.01         | Joback Method |
| dvisc         | 0.0008233 | Paxs    | 450.67          | Joback Method |
| dvisc         | 0.0003550 | Paxs    | 514.92          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001845 | Paxs | 579.17 | Joback Method |
| dvisc | 0.0001092 | Paxs | 643.42 | Joback Method |
| dvisc | 0.0000712 | Paxs | 707.68 | Joback Method |
| dvisc | 0.0000498 | Paxs | 771.93 | Joback Method |
| dvisc | 0.0000368 | Paxs | 836.18 | 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=U405336&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405336&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>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>logp:</b>               | Octanol/Water partition coefficient             |
| <b>m<sub>c</sub>vol:</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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