

# Glutaric acid, hept-2-yl isopropyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H28O4/c1-5-6-7-9-13(4)19-15(17)11-8-10-14(16)18-12(2)3/h12-13H,5-11H

TVRGGJGLVPECRV-UHFFFAOYSA-N

C15H28O4

CCCCC(C)OC(=O)CCCC(=O)OC(C)C

272.38

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -397.30 | kJ/mol  | Joback Method  |
| hf            | -853.09 | kJ/mol  | Joback Method  |
| hfus          | 33.13   | kJ/mol  | Joback Method  |
| hvap          | 66.52   | kJ/mol  | Joback Method  |
| log10ws       | -4.05   |         | Crippen Method |
| logp          | 3.620   |         | Crippen Method |
| mcvol         | 237.090 | ml/mol  | McGowan Method |
| pc            | 1537.87 | kPa     | Joback Method  |
| rinpol        | 1677.00 |         | NIST Webbook   |
| rinpol        | 1677.00 |         | NIST Webbook   |
| tb            | 694.30  | K       | Joback Method  |
| tc            | 874.56  | K       | Joback Method  |
| tf            | 373.13  | K       | Joback Method  |
| vc            | 0.911   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 678.23    | J/mol×K | 694.30          | Joback Method |
| cpg           | 694.81    | J/mol×K | 724.34          | Joback Method |
| cpg           | 710.56    | J/mol×K | 754.39          | Joback Method |
| cpg           | 725.49    | J/mol×K | 784.43          | Joback Method |
| cpg           | 739.62    | J/mol×K | 814.47          | Joback Method |
| cpg           | 752.95    | J/mol×K | 844.52          | Joback Method |
| cpg           | 765.47    | J/mol×K | 874.56          | Joback Method |
| dvisc         | 0.0020958 | Pa×s    | 373.13          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0008937 | Pa×s | 426.66 | Joback Method |
| dvisc | 0.0004608 | Pa×s | 480.19 | Joback Method |
| dvisc | 0.0002714 | Pa×s | 533.71 | Joback Method |
| dvisc | 0.0001760 | Pa×s | 587.24 | Joback Method |
| dvisc | 0.0001227 | Pa×s | 640.77 | Joback Method |
| dvisc | 0.0000905 | Pa×s | 694.30 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                         |
| <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=U393374&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393374&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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