

# Glutaric acid, isohexyl neopentyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C16H30O4/c1-13(2)8-7-11-19-14(17)9-6-10-15(18)20-12-16(3,4)5/h13H,6-12H

DPZIMINTVOHKMA-UHFFFAOYSA-N

C16H30O4

CC(C)CCCOC(=O)CCCC(=O)OCC(C)(C)C

286.41

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -383.60 | kJ/mol  | Joback Method  |
| hf            | -877.20 | kJ/mol  | Joback Method  |
| hfus          | 31.83   | kJ/mol  | Joback Method  |
| hvap          | 67.84   | kJ/mol  | Joback Method  |
| log10ws       | -3.76   |         | Crippen Method |
| logp          | 3.725   |         | Crippen Method |
| mcvol         | 251.180 | ml/mol  | McGowan Method |
| pc            | 1440.25 | kPa     | Joback Method  |
| rinpol        | 1843.00 |         | NIST Webbook   |
| tb            | 714.39  | K       | Joback Method  |
| tc            | 898.38  | K       | Joback Method  |
| tf            | 401.82  | K       | Joback Method  |
| vc            | 0.963   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 736.17    | J/mol×K | 714.39          | Joback Method |
| cpg           | 812.65    | J/mol×K | 867.72          | Joback Method |
| cpg           | 799.10    | J/mol×K | 837.05          | Joback Method |
| cpg           | 784.70    | J/mol×K | 806.39          | Joback Method |
| cpg           | 769.43    | J/mol×K | 775.72          | Joback Method |
| cpg           | 753.26    | J/mol×K | 745.06          | Joback Method |
| cpg           | 825.37    | J/mol×K | 898.38          | Joback Method |
| dvisc         | 0.0000715 | Pa×s    | 714.39          | Joback Method |
| dvisc         | 0.0000976 | Pa×s    | 662.30          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001406 | Pa×s | 610.20 | Joback Method |
| dvisc | 0.0002168 | Pa×s | 558.11 | Joback Method |
| dvisc | 0.0003656 | Pa×s | 506.01 | Joback Method |
| dvisc | 0.0006949 | Pa×s | 453.91 | Joback Method |
| dvisc | 0.0015604 | Pa×s | 401.82 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=U358343&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358343&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>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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