

# Glutaric acid, hex-4-yn-3-yl neopentyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C16H26O4/c1-6-9-13(7-2)20-15(18)11-8-10-14(17)19-12-16(3,4)5/h13H,7-8,10 |
| <b>InchiKey:</b>            | CWYIPKPQIOVVBI-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C16H26O4  |
| <b>SMILES:</b>              | CC#CC(CC)OC(=O)CCCC(=O)OCC(C)(C)C   |
| <b>Mol. weight [g/mol]:</b> | 282.38  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -180.80 | kJ/mol               | Joback Method  |
| hf            | -604.90 | kJ/mol               | Joback Method  |
| hfus          | 34.95   | kJ/mol               | Joback Method  |
| hvap          | 69.99   | kJ/mol               | Joback Method  |
| log10ws       | -3.91   |                      | Crippen Method |
| logp          | 3.091   |                      | Crippen Method |
| mvol          | 242.580 | ml/mol               | McGowan Method |
| pc            | 1632.49 | kPa                  | Joback Method  |
| rinpol        | 1812.00 |                      | NIST Webbook   |
| rinpol        | 1812.00 |                      | NIST Webbook   |
| tb            | 723.39  | K                    | Joback Method  |
| tc            | 922.55  | K                    | Joback Method  |
| tf            | 507.92  | K                    | Joback Method  |
| vc            | 0.924   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 690.74 | J/mol×K | 723.39          | Joback Method |
| cpg           | 707.30 | J/mol×K | 756.58          | Joback Method |
| cpg           | 722.91 | J/mol×K | 789.78          | Joback Method |
| cpg           | 737.56 | J/mol×K | 822.97          | Joback Method |
| cpg           | 751.30 | J/mol×K | 856.17          | Joback Method |
| cpg           | 764.13 | J/mol×K | 889.36          | Joback Method |
| cpg           | 776.09 | J/mol×K | 922.55          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=U391611&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391611&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>                                 |

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>hvp:</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>rinp:</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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