

Glutaric acid, ethyl nonyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C16H30O4/c1-3-5-6-7-8-9-10-14-20-16(18)13-11-12-15(17)19-4-2/h3-14H2,1-2 |
| InchiKey: | ZYYDWQNFSZRESV-UHFFFAOYSA-N |
| Formula: | C16H30O4 |
| SMILES: | CCCCCCCCCOC(=O)CCCC(=O)OCC |
| Mol. weight [g/mol]: | 286.41 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -384.00 | kJ/mol | Joback Method |
| hf | -863.17 | kJ/mol | Joback Method |
| hfus | 42.77 | kJ/mol | Joback Method |
| hvap | 69.52 | kJ/mol | Joback Method |
| log10ws | -4.25 | | Crippen Method |
| logp | 4.014 | | Crippen Method |
| mcvol | 251.180 | ml/mol | McGowan Method |
| pc | 1411.18 | kPa | Joback Method |
| rinpola | 2001.00 | | NIST Webbook |
| tb | 718.06 | K | Joback Method |
| tc | 894.33 | K | Joback Method |
| tf | 414.40 | K | Joback Method |
| vc | 0.980 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 733.60 | J/molxK | 718.06 | Joback Method |
| cpg | 750.17 | J/molxK | 747.44 | Joback Method |
| cpg | 765.92 | J/molxK | 776.82 | Joback Method |
| cpg | 780.87 | J/molxK | 806.19 | Joback Method |
| cpg | 795.02 | J/molxK | 835.57 | Joback Method |
| cpg | 808.37 | J/molxK | 864.95 | Joback Method |
| cpg | 820.95 | J/molxK | 894.33 | Joback Method |
| dvisc | 0.0012551 | Paxs | 414.40 | Joback Method |
| dvisc | 0.0006418 | Paxs | 465.01 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003744 | Paxs | 515.62 | Joback Method |
| dvisc | 0.0002405 | Paxs | 566.23 | Joback Method |
| dvisc | 0.0001661 | Paxs | 616.84 | Joback Method |
| dvisc | 0.0001214 | Paxs | 667.45 | Joback Method |
| dvisc | 0.0000927 | Paxs | 718.06 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U358276&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/67-324-8/Glutaric-acid-ethyl-nonyl-ester.pdf>

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