

Diglycolic acid, ethyl oct-4-yl ester

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C14H26O5/c1-4-7-9-12(8-5-2)19-14(16)11-17-10-13(15)18-6-3/h12H,4-11H2,1 |
| InchiKey: | GCTJNSSXNRHRJS-UHFFFAOYSA-N |
| Formula: | C14H26O5 |
| SMILES: | CCCCC(CCC)OC(=O)COCC(=O)OCC |
| Mol. weight [g/mol]: | 274.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -508.28 | kJ/mol | Joback Method |
| hf | -959.39 | kJ/mol | Joback Method |
| hfus | 35.25 | kJ/mol | Joback Method |
| hvap | 67.09 | kJ/mol | Joback Method |
| log10ws | -2.61 | | Crippen Method |
| logp | 2.468 | | Crippen Method |
| mcvol | 228.870 | ml/mol | McGowan Method |
| pc | 1627.22 | kPa | Joback Method |
| rinpola | 2105.00 | | NIST Webbook |
| rinpola | 2105.00 | | NIST Webbook |
| tb | 694.28 | K | Joback Method |
| tc | 872.83 | K | Joback Method |
| tf | 399.09 | K | Joback Method |
| vc | 0.879 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 651.48 | J/molxK | 694.28 | Joback Method |
| cpg | 667.16 | J/molxK | 724.04 | Joback Method |
| cpg | 682.08 | J/molxK | 753.80 | Joback Method |
| cpg | 696.23 | J/molxK | 783.56 | Joback Method |
| cpg | 709.61 | J/molxK | 813.32 | Joback Method |
| cpg | 722.22 | J/molxK | 843.08 | Joback Method |
| cpg | 734.04 | J/molxK | 872.83 | Joback Method |
| dvisc | 0.0012554 | Paxs | 399.09 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0006269 | Paxs | 448.29 | Joback Method |
| dvisc | 0.0003592 | Paxs | 497.49 | Joback Method |
| dvisc | 0.0002275 | Paxs | 546.68 | Joback Method |
| dvisc | 0.0001553 | Paxs | 595.88 | Joback Method |
| dvisc | 0.0001124 | Paxs | 645.08 | Joback Method |
| dvisc | 0.0000852 | Paxs | 694.28 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=U382017&Units=SI |

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 |

Latest version available from:

<https://www.chemeo.com/cid/89-980-6/Diglycolic-acid-ethyl-oct-4-yl-ester.pdf>

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