

Diethyl propane-1,3-diyl dicarbonate

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|-----------------------------|--|
| Inchi: | InChI=1S/C9H16O6/c1-3-12-8(10)14-6-5-7-15-9(11)13-4-2/h3-7H2,1-2H3 |
| InchiKey: | OFOLPWWHUDBNSD-UHFFFAOYSA-N |
| Formula: | C9H16O6 |
| SMILES: | CCOC(=O)OCCOC(=O)OCC |
| Mol. weight [g/mol]: | 220.22 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -652.94 | kJ/mol | Joback Method |
| hf | -983.13 | kJ/mol | Joback Method |
| hfus | 27.02 | kJ/mol | Joback Method |
| hvap | 58.76 | kJ/mol | Joback Method |
| log10ws | -1.45 | | Crippen Method |
| logp | 1.723 | | Crippen Method |
| mcvol | 164.290 | ml/mol | McGowan Method |
| pc | 2441.06 | kPa | Joback Method |
| rinsol | 1432.00 | | NIST Webbook |
| tb | 602.74 | K | Joback Method |
| tc | 782.89 | K | Joback Method |
| tf | 379.97 | K | Joback Method |
| vc | 0.624 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 417.67 | J/molxK | 602.74 | Joback Method |
| cpg | 429.90 | J/molxK | 632.77 | Joback Method |
| cpg | 441.68 | J/molxK | 662.79 | Joback Method |
| cpg | 452.97 | J/molxK | 692.82 | Joback Method |
| cpg | 463.77 | J/molxK | 722.84 | Joback Method |
| cpg | 474.04 | J/molxK | 752.87 | Joback Method |
| cpg | 483.77 | J/molxK | 782.89 | Joback Method |
| dvisc | 0.0010531 | Paxs | 379.97 | Joback Method |
| dvisc | 0.0006381 | Paxs | 417.10 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0004196 | Paxs | 454.23 | Joback Method |
| dvisc | 0.0002940 | Paxs | 491.36 | Joback Method |
| dvisc | 0.0002166 | Paxs | 528.48 | Joback Method |
| dvisc | 0.0001660 | Paxs | 565.61 | Joback Method |
| dvisc | 0.0001315 | Paxs | 602.74 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373779&Units=SI |
| 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 |

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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