

Carbonic acid, ethyl cyclohexyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C9H16O3/c1-2-11-9(10)12-8-6-4-3-5-7-8/h8H,2-7H2,1H3 |
| InchiKey: | XSSAWOIEQNZRDP-UHFFFAOYSA-N |
| Formula: | C9H16O3 |
| SMILES: | CCOC(=O)OC1CCCCC1 |
| Mol. weight [g/mol]: | 172.22 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -289.57 | kJ/mol | Joback Method |
| hf | -551.79 | kJ/mol | Joback Method |
| hfus | 14.88 | kJ/mol | Joback Method |
| hvap | 47.62 | kJ/mol | Joback Method |
| log10ws | -2.52 | | Crippen Method |
| logp | 2.492 | | Crippen Method |
| mcvol | 140.120 | ml/mol | McGowan Method |
| pc | 2928.17 | kPa | Joback Method |
| rinsol | 1219.00 | | NIST Webbook |
| tb | 523.58 | K | Joback Method |
| tc | 730.09 | K | Joback Method |
| tf | 292.96 | K | Joback Method |
| vc | 0.514 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 334.41 | J/molxK | 523.58 | Joback Method |
| cpg | 409.89 | J/molxK | 695.68 | Joback Method |
| cpg | 396.36 | J/molxK | 661.26 | Joback Method |
| cpg | 382.04 | J/molxK | 626.84 | Joback Method |
| cpg | 366.95 | J/molxK | 592.42 | Joback Method |
| cpg | 351.07 | J/molxK | 558.00 | Joback Method |
| cpg | 422.62 | J/molxK | 730.09 | Joback Method |
| dvisc | 0.0002146 | Paxs | 523.58 | Joback Method |
| dvisc | 0.0002806 | Paxs | 485.14 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003842 | Paxs | 446.71 | Joback Method |
| dvisc | 0.0005583 | Paxs | 408.27 | Joback Method |
| dvisc | 0.0008766 | Paxs | 369.83 | Joback Method |
| dvisc | 0.0015283 | Paxs | 331.40 | Joback Method |
| dvisc | 0.0030831 | Paxs | 292.96 | 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=U357913&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 |
| mccvol: | 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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