

Carbonic acid, (1R)-(-)-menthyl hexyl ester

Inchi: InChI=1S/C17H32O3/c1-5-6-7-8-11-19-17(18)20-16-12-15(13(2)3)10-9-14(16)4/h13-16H
InchiKey: YMKMWFFBPKMXHW-UHFFFAOYSA-N
Formula: C17H32O3
SMILES: CCCCCCOC(=O)OC1CC(C(C)C)CCC1C
Mol. weight [g/mol]: 284.43

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -240.07 | kJ/mol | Joback Method |
| hf | -762.87 | kJ/mol | Joback Method |
| hfus | 34.21 | kJ/mol | Joback Method |
| hvap | 64.42 | kJ/mol | Joback Method |
| log10ws | -5.15 | | Crippen Method |
| logp | 5.181 | | Crippen Method |
| mvol | 252.840 | ml/mol | McGowan Method |
| pc | 1398.55 | kPa | Joback Method |
| rinpol | 1854.00 | | NIST Webbook |
| rinpol | 1854.00 | | NIST Webbook |
| tb | 696.84 | K | Joback Method |
| tc | 887.15 | K | Joback Method |
| tf | 359.64 | K | Joback Method |
| vc | 0.955 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 763.95 | J/mol×K | 696.84 | Joback Method |
| cpg | 785.35 | J/mol×K | 728.56 | Joback Method |
| cpg | 805.58 | J/mol×K | 760.28 | Joback Method |
| cpg | 824.65 | J/mol×K | 792.00 | Joback Method |
| cpg | 842.57 | J/mol×K | 823.72 | Joback Method |
| cpg | 859.34 | J/mol×K | 855.44 | Joback Method |
| cpg | 874.96 | J/mol×K | 887.15 | Joback Method |
| dvisc | 0.0019351 | Paxs | 359.64 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0008895 | Paxs | 415.84 | Joback Method |
| dvisc | 0.0004920 | Paxs | 472.04 | Joback Method |
| dvisc | 0.0003087 | Paxs | 528.24 | Joback Method |
| dvisc | 0.0002118 | Paxs | 584.44 | Joback Method |
| dvisc | 0.0001553 | Paxs | 640.64 | Joback Method |
| dvisc | 0.0001197 | Paxs | 696.84 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392435&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 |
| 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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<https://www.chemeo.com/cid/90-356-7/Carbonic-acid-1R-menthyl-hexyl-ester.pdf>

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