# Carbonic acid, di(2-ethylhexyl) ester

**Other names:** bis(2-ethylhexyl) carbonate
**Inchi:** InChI=1S/C17H34O3/c1-5-9-11-15(7-3)13-19-17(18)20-14-16(8-4)12-10-6-2/h15-16H,5-1
**InchiKey:** PXTQQOLKZBLYDY-UHFFFAOYSA-N
**Formula:** C17H34O3
**SMILES:** CCCCC(CC)COC(=O)OCC(CC)CCCC
**Mol. weight [g/mol]:** 286.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.8145 | | Cheméo Relay (1.0) |
| hf | -900.07 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 36.71 | kJ/mol | Joback Method |
| hvap | 89.12 | kJ/mol | Cheméo Relay (1.0) |
| log10ws | -5.51 | | Cheméo Relay (1.0) |
| logp | 5.572 | | Crippen Method |
| mcvol | 263.700 | ml/mol | McGowan Method |
| pc | 1270.97 | kPa | Joback Method |
| tb | 579.94 | K | Cheméo Relay (1.0) |
| tc | 716.47 | K | Cheméo Relay (1.0) |
| tf | 192.72 | K | Cheméo Relay (1.0) |
| vc | 0.981 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 764.61 | J/mol×K | 686.19 | Joback Method |
| cpg | 783.21 | J/mol×K | 714.92 | Joback Method |
| cpg | 800.96 | J/mol×K | 743.66 | Joback Method |
| cpg | 817.88 | J/mol×K | 772.39 | Joback Method |
| cpg | 833.97 | J/mol×K | 801.13 | Joback Method |
| cpg | 849.24 | J/mol×K | 829.86 | Joback Method |
| cpg | 863.71 | J/mol×K | 858.60 | Joback Method |
| dvisc | 0.0024947 | Pa×s | 345.74 | Joback Method |
| dvisc | 0.0009085 | Pa×s | 402.48 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0004247 | Pa×s | 459.22 | Joback Method |
| dvisc | 0.0002347 | Pa×s | 515.96 | Joback Method |
| dvisc | 0.0001458 | Pa×s | 572.71 | Joback Method |
| dvisc | 0.0000987 | Pa×s | 629.45 | Joback Method |
| dvisc | 0.0000713 | Pa×s | 686.19 | Joback Method |

# Sources

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C14858732&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

# Legend

**af:** Acentric Factor
**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**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
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume