# OCTANOIC ACID, CYCLOHEXYL ESTER

**Other names:** Cyclohexyl caprylate
**Inchi:** InChI=1S/C14H26O2/c1-2-3-4-5-9-12-14(15)16-13-10-7-6-8-11-13/h13H,2-12H2,1H3
**InchiKey:** TXWXLLMVRVKQSO-UHFFFAOYSA-N
**Formula:** C14H26O2
**SMILES:** CCCCCCCC(=O)OC1CCCCC1
**Mol. weight [g/mol]:** 226.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.6593 | | Cheméo Relay (1.0) |
| hf | -615.71 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 26.64 | kJ/mol | Joback Method |
| hvap | 73.94 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.62 | eV | Cheméo Relay (1.0) |
| log10ws | -4.55 | | Cheméo Relay (1.0) |
| logp | 4.223 | | Crippen Method |
| mcvol | 204.700 | ml/mol | McGowan Method |
| pc | 1872.41 | kPa | Joback Method |
| rinpol | 1600.00 | | NIST Webbook |
| rinpol | 1600.00 | | NIST Webbook |
| tb | 548.85 | K | Cheméo Relay (1.0) |
| tc | 756.68 | K | Cheméo Relay (1.0) |
| tf | 247.96 | K | Cheméo Relay (1.0) |
| vc | 0.767 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 559.97 | J/mol×K | 615.56 | Joback Method |
| cpg | 664.38 | J/mol×K | 809.77 | Joback Method |
| cpg | 649.42 | J/mol×K | 777.41 | Joback Method |
| cpg | 633.51 | J/mol×K | 745.04 | Joback Method |
| cpg | 616.63 | J/mol×K | 712.67 | Joback Method |
| cpg | 598.76 | J/mol×K | 680.30 | Joback Method |

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|---|---|---|---|---|
| cpg | 579.88 | J/mol×K | 647.93 | Joback Method |
| dvisc | 0.0004679 | Pa×s | 471.32 | Joback Method |
| dvisc | 0.0001630 | Pa×s | 615.56 | Joback Method |
| dvisc | 0.0002182 | Pa×s | 567.48 | Joback Method |
| dvisc | 0.0003085 | Pa×s | 519.40 | Joback Method |
| dvisc | 0.0034050 | Pa×s | 327.08 | Joback Method |
| dvisc | 0.0007802 | Pa×s | 423.24 | Joback Method |
| dvisc | 0.0014830 | Pa×s | 375.16 | Joback Method |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1551424&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

# 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
**ie:** Ionization energy
**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