# OCTANOIC ACID, 8-CHLORO-8-OXO-, ETHYL ESTER

**Other names:** Ethyl 8-chloro-8-oxooctanoate
ethyl 7-chloro-7-formylheptanoate
**Inchi:** InChI=1S/C10H17ClO3/c1-2-14-10(13)8-6-4-3-5-7-9(11)12/h2-8H2,1H3
**InchiKey:** ZKXJSBHGOFAICL-UHFFFAOYSA-N
**Formula:** C10H17ClO3
**SMILES:** CCOC(=O)CCCCCCC(=O)Cl
**Mol. weight [g/mol]:** 220.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.6660 | | Cheméo Relay (1.0) |
| gf | -341.45 | kJ/mol | Joback Method |
| hf | -717.51 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 30.24 | kJ/mol | Joback Method |
| hvap | 68.49 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.74 | eV | Cheméo Relay (1.0) |
| log10ws | -3.09 | | Cheméo Relay (1.0) |
| logp | 2.656 | | Crippen Method |
| mcvol | 173.010 | ml/mol | McGowan Method |
| pc | 2254.67 | kPa | Joback Method |
| rinpol | 1513.00 | | NIST Webbook |
| tb | 526.82 | K | Cheméo Relay (1.0) |
| tc | 697.72 | K | Cheméo Relay (1.0) |
| tf | 273.97 | K | Cheméo Relay (1.0) |
| vc | 0.647 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 418.29 | J/mol×K | 595.79 | Joback Method |
| cpg | 431.00 | J/mol×K | 626.70 | Joback Method |
| cpg | 443.12 | J/mol×K | 657.61 | Joback Method |
| cpg | 454.65 | J/mol×K | 688.52 | Joback Method |
| cpg | 465.61 | J/mol×K | 719.43 | Joback Method |

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|---|---|---|---|---|
| cpg | 476.00 | J/mol×K | 750.34 | Joback Method |
| cpg | 485.83 | J/mol×K | 781.25 | Joback Method |
| dvisc | 0.0023152 | Pa×s | 354.47 | Joback Method |
| dvisc | 0.0012887 | Pa×s | 394.69 | Joback Method |
| dvisc | 0.0007995 | Pa×s | 434.91 | Joback Method |
| dvisc | 0.0005377 | Pa×s | 475.13 | Joback Method |
| dvisc | 0.0003847 | Pa×s | 515.35 | Joback Method |
| dvisc | 0.0002890 | Pa×s | 555.57 | Joback Method |
| dvisc | 0.0002256 | Pa×s | 595.79 | Joback Method |

# Sources

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|---|---|
| **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):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C14113021&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **af:** | Acentric Factor |
| **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 |
| **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