# Octyl 4-chlorobutanoate

**Other names:** Butanoic acid, 4-chloro, octyl ester
**Inchi:** InChI=1S/C12H23ClO2/c1-2-3-4-5-6-7-11-15-12(14)9-8-10-13/h2-11H2,1H3
**InchiKey:** JLYKWKRZFITWIT-UHFFFAOYSA-N
**Formula:** C12H23ClO2
**SMILES:** CCCCCCCCOC(=O)CCCCl
**Mol. weight [g/mol]:** 234.76

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -195.69 | kJ/mol | Joback Method |
| hf | -551.55 | kJ/mol | Joback Method |
| hfus | 33.82 | kJ/mol | Joback Method |
| hvap | 55.85 | kJ/mol | Joback Method |
| log10ws | -3.86 | | Crippen Method |
| logp | 3.909 | | Crippen Method |
| mcvol | 199.620 | ml/mol | McGowan Method |
| pc | 1793.94 | kPa | Joback Method |
| rinpol | 1619.00 | | NIST Webbook |
| rinpol | 1605.00 | | NIST Webbook |
| rinpol | 1605.00 | | NIST Webbook |
| rinpol | 1619.00 | | NIST Webbook |
| rinpol | 1599.00 | | NIST Webbook |
| rinpol | 1601.00 | | NIST Webbook |
| rinpol | 1607.00 | | NIST Webbook |
| rinpol | 1611.00 | | NIST Webbook |
| tb | 587.68 | K | Joback Method |
| tc | 762.26 | K | Joback Method |
| tf | 327.08 | K | Joback Method |
| vc | 0.780 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 496.42 | J/mol×K | 587.68 | Joback Method |

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|---|---|---|---|---|
| cpg | 511.47 | J/mol×K | 616.78 | Joback Method |
| cpg | 525.87 | J/mol×K | 645.87 | Joback Method |
| cpg | 539.64 | J/mol×K | 674.97 | Joback Method |
| cpg | 552.80 | J/mol×K | 704.07 | Joback Method |
| cpg | 565.36 | J/mol×K | 733.17 | Joback Method |
| cpg | 577.32 | J/mol×K | 762.26 | Joback Method |
| dvisc | 0.0026085 | Pa×s | 327.08 | Joback Method |
| dvisc | 0.0012830 | Pa×s | 370.51 | Joback Method |
| dvisc | 0.0007323 | Pa×s | 413.95 | Joback Method |
| dvisc | 0.0004650 | Pa×s | 457.38 | Joback Method |
| dvisc | 0.0003194 | Pa×s | 500.81 | Joback Method |
| dvisc | 0.0002330 | Pa×s | 544.25 | Joback Method |
| dvisc | 0.0001781 | Pa×s | 587.68 | Joback Method |

# Sources

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

**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=R28380&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

**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