# 4-Chlorobutyric acid, eicosyl ester

**Inchi:** InChI=1S/C24H47ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-27-24(26)
**InchiKey:** RROXGHSGTRLUSS-UHFFFAOYSA-N
**Formula:** C24H47ClO2
**SMILES:** CCCCCCCCCCCCCCCCCCCCOC(=O)CCCCl
**Mol. weight [g/mol]:** 403.08

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -94.65 | kJ/mol | Joback Method |
| hf | -799.23 | kJ/mol | Joback Method |
| hfus | 64.90 | kJ/mol | Joback Method |
| hvap | 82.56 | kJ/mol | Joback Method |
| log10ws | -8.88 | | Crippen Method |
| logp | 8.590 | | Crippen Method |
| mcvol | 368.700 | ml/mol | McGowan Method |
| pc | 810.30 | kPa | Joback Method |
| rinpol | 2871.00 | | NIST Webbook |
| rinpol | 2871.00 | | NIST Webbook |
| tb | 862.24 | K | Joback Method |
| tc | 1055.83 | K | Joback Method |
| tf | 462.32 | K | Joback Method |
| vc | 1.452 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1192.29 | J/mol×K | 862.24 | Joback Method |
| cpg | 1213.20 | J/mol×K | 894.51 | Joback Method |
| cpg | 1232.89 | J/mol×K | 926.77 | Joback Method |
| cpg | 1251.41 | J/mol×K | 959.04 | Joback Method |
| cpg | 1268.80 | J/mol×K | 991.30 | Joback Method |
| cpg | 1285.11 | J/mol×K | 1023.57 | Joback Method |
| cpg | 1300.39 | J/mol×K | 1055.83 | Joback Method |
| dvisc | 0.0008062 | Pa×s | 462.32 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003454 | Pa×s | 528.97 | Joback Method |
| dvisc | 0.0001789 | Pa×s | 595.63 | Joback Method |
| dvisc | 0.0001058 | Pa×s | 662.28 | Joback Method |
| dvisc | 0.0000689 | Pa×s | 728.93 | Joback Method |
| dvisc | 0.0000482 | Pa×s | 795.59 | Joback Method |
| dvisc | 0.0000356 | Pa×s | 862.24 | Joback Method |

# Sources

**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=U340236&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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