# 3-Chloropropionic acid, octadecyl ester

**Other names:** Propanoic acid, 3-chloro, octadecyl ester
**Inchi:** InChI=1S/C21H41ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-24-21(23)18-19-
**InchiKey:** IWNDNJGFFCNPKN-UHFFFAOYSA-N
**Formula:** C21H41ClO2
**SMILES:** CCCCCCCCCCCCCCCCCCOC(=O)CCCl
**Mol. weight [g/mol]:** 361.00
**CAS:** 88168-99-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -119.91 | kJ/mol | Joback Method |
| hf | -737.31 | kJ/mol | Joback Method |
| hfus | 57.13 | kJ/mol | Joback Method |
| hvap | 75.88 | kJ/mol | Joback Method |
| log10ws | -7.63 | | Crippen Method |
| logp | 7.420 | | Crippen Method |
| mcvol | 326.430 | ml/mol | McGowan Method |
| pc | 961.48 | kPa | Joback Method |
| rinpol | 2499.00 | | NIST Webbook |
| rinpol | 2504.00 | | NIST Webbook |
| rinpol | 2511.00 | | NIST Webbook |
| rinpol | 2499.00 | | NIST Webbook |
| rinpol | 2516.00 | | NIST Webbook |
| ripol | 2983.00 | | NIST Webbook |
| ripol | 2983.00 | | NIST Webbook |
| ripol | 3006.00 | | NIST Webbook |
| ripol | 3015.00 | | NIST Webbook |
| tb | 793.60 | K | Joback Method |
| tc | 973.90 | K | Joback Method |
| tf | 428.51 | K | Joback Method |
| vc | 1.284 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1005.07 | J/mol×K | 793.60 | Joback Method |
| cpg | 1024.39 | J/mol×K | 823.65 | Joback Method |
| cpg | 1042.70 | J/mol×K | 853.70 | Joback Method |
| cpg | 1060.04 | J/mol×K | 883.75 | Joback Method |
| cpg | 1076.44 | J/mol×K | 913.80 | Joback Method |
| cpg | 1091.93 | J/mol×K | 943.85 | Joback Method |
| cpg | 1106.54 | J/mol×K | 973.90 | Joback Method |
| dvisc | 0.0011536 | Pa×s | 428.51 | Joback Method |
| dvisc | 0.0005079 | Pa×s | 489.36 | Joback Method |
| dvisc | 0.0002681 | Pa×s | 550.21 | Joback Method |
| dvisc | 0.0001607 | Pa×s | 611.05 | Joback Method |
| dvisc | 0.0001057 | Pa×s | 671.90 | Joback Method |
| dvisc | 0.0000745 | Pa×s | 732.75 | Joback Method |
| dvisc | 0.0000554 | Pa×s | 793.60 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C88168994&Units=SI
**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

# 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
**ripol:** Polar retention indices

| | |
|---|---|
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |