# Fumaric acid, 2-chloropropyl undecyl ester

**Inchi:** InChI=1S/C18H31ClO4/c1-3-4-5-6-7-8-9-10-11-14-22-17(20)12-13-18(21)23-15-16(2)19/
**InchiKey:** PJJXMPHMXBTGDX-OUKQBFOZSA-N
**Formula:** C18H31ClO4
**SMILES:** CCCCCCCCCCCOC(=O)C=CC(=O)OCC(C)Cl
**Mol. weight [g/mol]:** 346.89

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -301.31 | kJ/mol | Joback Method |
| hf | -808.25 | kJ/mol | Joback Method |
| hfus | 48.83 | kJ/mol | Joback Method |
| hvap | 77.93 | kJ/mol | Joback Method |
| log10ws | -5.20 | | Crippen Method |
| logp | 4.787 | | Crippen Method |
| mcvol | 287.300 | ml/mol | McGowan Method |
| pc | 1247.73 | kPa | Joback Method |
| rinpol | 2375.00 | | NIST Webbook |
| rinpol | 2375.00 | | NIST Webbook |
| tb | 804.97 | K | Joback Method |
| tc | 994.12 | K | Joback Method |
| tf | 446.78 | K | Joback Method |
| vc | 1.115 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 856.22 | J/mol×K | 804.97 | Joback Method |
| cpg | 927.52 | J/mol×K | 962.59 | Joback Method |
| cpg | 915.05 | J/mol×K | 931.07 | Joback Method |
| cpg | 901.70 | J/mol×K | 899.54 | Joback Method |
| cpg | 887.47 | J/mol×K | 868.02 | Joback Method |
| cpg | 872.31 | J/mol×K | 836.49 | Joback Method |
| cpg | 939.15 | J/mol×K | 994.12 | Joback Method |
| dvisc | 0.0000489 | Pa×s | 804.97 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000654 | Pa×s | 745.27 | Joback Method |
| dvisc | 0.0000920 | Pa×s | 685.57 | Joback Method |
| dvisc | 0.0001383 | Pa×s | 625.88 | Joback Method |
| dvisc | 0.0002265 | Pa×s | 566.18 | Joback Method |
| dvisc | 0.0004166 | Pa×s | 506.48 | Joback Method |
| dvisc | 0.0009018 | Pa×s | 446.78 | Joback Method |

# Sources

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|---|---|
| **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=U348569&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |