# Phthalic acid, 2-chloropropyl ethyl ester

**Inchi:** InChI=1S/C13H15ClO4/c1-3-17-12(15)10-6-4-5-7-11(10)13(16)18-8-9(2)14/h4-7,9H,3,8H
**InchiKey:** YFHRWQJTTKJKPE-UHFFFAOYSA-N
**Formula:** C13H15ClO4
**SMILES:** CCOC(=O)c1ccccc1C(=O)OCC(C)Cl
**Mol. weight [g/mol]:** 270.71

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -320.85 | kJ/mol | Joback Method |
| hf | -597.21 | kJ/mol | Joback Method |
| hfus | 29.33 | kJ/mol | Joback Method |
| hvap | 69.78 | kJ/mol | Joback Method |
| log10ws | -3.48 | | Crippen Method |
| logp | 2.647 | | Crippen Method |
| mcvol | 197.390 | ml/mol | McGowan Method |
| pc | 2295.91 | kPa | Joback Method |
| rinpol | 1868.00 | | NIST Webbook |
| tb | 718.07 | K | Joback Method |
| tc | 933.75 | K | Joback Method |
| tf | 434.45 | K | Joback Method |
| vc | 0.747 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 513.64 | J/mol×K | 718.07 | Joback Method |
| cpg | 570.15 | J/mol×K | 897.80 | Joback Method |
| cpg | 560.66 | J/mol×K | 861.85 | Joback Method |
| cpg | 550.27 | J/mol×K | 825.91 | Joback Method |
| cpg | 538.97 | J/mol×K | 789.96 | Joback Method |
| cpg | 526.77 | J/mol×K | 754.02 | Joback Method |
| cpg | 578.75 | J/mol×K | 933.75 | Joback Method |
| dvisc | 0.0001127 | Pa×s | 718.07 | Joback Method |
| dvisc | 0.0001435 | Pa×s | 670.80 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001896 | Pa×s | 623.53 | Joback Method |
| dvisc | 0.0002621 | Pa×s | 576.26 | Joback Method |
| dvisc | 0.0003839 | Pa×s | 528.99 | Joback Method |
| dvisc | 0.0006062 | Pa×s | 481.72 | Joback Method |
| dvisc | 0.0010572 | Pa×s | 434.45 | Joback Method |

# Sources

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|---|---|
| **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=U356822&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 |