# Phthalic acid, 2,2-dichloroethyl dodecyl ester

**Inchi:** InChI=1S/C22H32Cl2O4/c1-2-3-4-5-6-7-8-9-10-13-16-27-21(25)18-14-11-12-15-19(18)22
**InchiKey:** BJDHUPJZEJEDDL-UHFFFAOYSA-N
**Formula:** C22H32Cl2O4
**SMILES:** CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(Cl)Cl
**Mol. weight [g/mol]:** 431.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -257.00 | kJ/mol | Joback Method |
| hf | -798.71 | kJ/mol | Joback Method |
| hfus | 56.83 | kJ/mol | Joback Method |
| hvap | 94.20 | kJ/mol | Joback Method |
| log10ws | -7.89 | | Crippen Method |
| logp | 6.725 | | Crippen Method |
| mcvol | 336.440 | ml/mol | McGowan Method |
| pc | 1120.05 | kPa | Joback Method |
| rinpol | 2925.00 | | NIST Webbook |
| rinpol | 2925.00 | | NIST Webbook |
| tb | 961.42 | K | Joback Method |
| tc | 1178.64 | K | Joback Method |
| tf | 565.80 | K | Joback Method |
| vc | 1.300 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1049.78 | J/mol×K | 961.42 | Joback Method |
| cpg | 1063.99 | J/mol×K | 997.62 | Joback Method |
| cpg | 1076.90 | J/mol×K | 1033.83 | Joback Method |
| cpg | 1088.54 | J/mol×K | 1070.03 | Joback Method |
| cpg | 1098.95 | J/mol×K | 1106.23 | Joback Method |
| cpg | 1108.17 | J/mol×K | 1142.44 | Joback Method |
| cpg | 1116.24 | J/mol×K | 1178.64 | Joback Method |
| dvisc | 0.0003401 | Pa×s | 565.80 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001789 | Pa×s | 631.74 | Joback Method |
| dvisc | 0.0001063 | Pa×s | 697.67 | Joback Method |
| dvisc | 0.0000691 | Pa×s | 763.61 | Joback Method |
| dvisc | 0.0000481 | Pa×s | 829.55 | Joback Method |
| dvisc | 0.0000353 | Pa×s | 895.48 | Joback Method |
| dvisc | 0.0000270 | Pa×s | 961.42 | Joback Method |

# Sources

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|---|---|
| **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=U356933&Units=SI |

# 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 |