# Terephthalic acid, 2-chloropropyl pentadecyl ester

**Inchi:** InChI=1S/C26H41ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-20-30-25(28)23-16-18-24(19

**InchiKey:** ZPXCFBKQDGASQP-UHFFFAOYSA-N

**Formula:** C26H41ClO4

**SMILES:** CCCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(C)Cl)cc1

**Mol. weight [g/mol]:** 453.05

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -211.39 | kJ/mol | Joback Method |
| hf | -865.53 | kJ/mol | Joback Method |
| hfus | 63.00 | kJ/mol | Joback Method |
| hvap | 98.72 | kJ/mol | Joback Method |
| log10ws | -8.92 | | Crippen Method |
| logp | 7.719 | | Crippen Method |
| mcvol | 380.560 | ml/mol | McGowan Method |
| pc | 899.10 | kPa | Joback Method |
| rinpol | 3298.00 | | NIST Webbook |
| rinpol | 3298.00 | | NIST Webbook |
| tb | 1015.51 | K | Joback Method |
| tc | 1244.39 | K | Joback Method |
| tf | 580.96 | K | Joback Method |
| vc | 1.474 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1270.07 | J/mol×K | 1015.51 | Joback Method |
| cpg | 1336.12 | J/mol×K | 1206.24 | Joback Method |
| cpg | 1325.88 | J/mol×K | 1168.10 | Joback Method |
| cpg | 1314.22 | J/mol×K | 1129.95 | Joback Method |
| cpg | 1301.07 | J/mol×K | 1091.80 | Joback Method |
| cpg | 1286.37 | J/mol×K | 1053.66 | Joback Method |
| cpg | 1345.00 | J/mol×K | 1244.39 | Joback Method |
| dvisc | 0.0000174 | Pa×s | 1015.51 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000229 | Pa×s | 943.08 | Joback Method |
| dvisc | 0.0000317 | Pa×s | 870.66 | Joback Method |
| dvisc | 0.0000466 | Pa×s | 798.23 | Joback Method |
| dvisc | 0.0000739 | Pa×s | 725.81 | Joback Method |
| dvisc | 0.0001298 | Pa×s | 653.38 | Joback Method |
| dvisc | 0.0002622 | Pa×s | 580.96 | Joback Method |

# Sources

| | |
|---|---|
| **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=U356180&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |

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