# Phthalic acid, di(2,4,5-trichlorophenyl) ester

**Inchi:** InChI=1S/C20H8Cl6O4/c21-11-5-15(25)17(7-13(11)23)29-19(27)9-3-1-2-4-10(9)20(28)30
**InchiKey:** WIUYPBXSBMKVDU-UHFFFAOYSA-N
**Formula:** C20H8Cl6O4
**SMILES:** O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1ccccc1C(=O)Oc1cc(Cl)c(Cl)cc1Cl
**Mol. weight [g/mol]:** 524.99

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -152.08 | kJ/mol | Joback Method |
| hf | -410.87 | kJ/mol | Joback Method |
| hfus | 57.71 | kJ/mol | Joback Method |
| hvap | 116.20 | kJ/mol | Joback Method |
| log10ws | -9.76 | | Crippen Method |
| logp | 8.045 | | Crippen Method |
| mcvol | 309.700 | ml/mol | McGowan Method |
| pc | 1765.41 | kPa | Joback Method |
| rinpol | 3555.00 | | NIST Webbook |
| rinpol | 3555.00 | | NIST Webbook |
| tb | 1149.06 | K | Joback Method |
| tc | 1424.67 | K | Joback Method |
| tf | 805.90 | K | Joback Method |
| vc | 1.173 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 756.19 | J/mol×K | 1149.06 | Joback Method |
| cpg | 758.22 | J/mol×K | 1195.00 | Joback Method |
| cpg | 758.76 | J/mol×K | 1240.93 | Joback Method |
| cpg | 757.85 | J/mol×K | 1286.87 | Joback Method |
| cpg | 755.50 | J/mol×K | 1332.80 | Joback Method |
| cpg | 751.76 | J/mol×K | 1378.74 | Joback Method |
| cpg | 746.66 | J/mol×K | 1424.67 | Joback Method |
| dvisc | 0.0001010 | Pa×s | 805.90 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000745 | Pa×s | 863.09 | Joback Method |
| dvisc | 0.0000571 | Pa×s | 920.29 | Joback Method |
| dvisc | 0.0000451 | Pa×s | 977.48 | Joback Method |
| dvisc | 0.0000366 | Pa×s | 1034.67 | Joback Method |
| dvisc | 0.0000304 | Pa×s | 1091.87 | Joback Method |
| dvisc | 0.0000257 | Pa×s | 1149.06 | 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=U357053&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 |