# Diethylmalonic acid, di(4-chloro-3-methylphenyl) ester

**Inchi:** InChI=1S/C21H22Cl2O4/c1-5-21(6-2,19(24)26-15-7-9-17(22)13(3)11-15)20(25)27-16-8-1

**InchiKey:** XUMFIUJWHHLVEF-UHFFFAOYSA-N

**Formula:** C21H22Cl2O4

**SMILES:** CCC(CC)(C(=O)Oc1ccc(Cl)c(C)c1)C(=O)Oc1ccc(Cl)c(C)c1

**Mol. weight [g/mol]:** 409.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -176.62 | kJ/mol | Joback Method |
| hf | -579.42 | kJ/mol | Joback Method |
| hfus | 43.23 | kJ/mol | Joback Method |
| hvap | 95.33 | kJ/mol | Joback Method |
| log10ws | -7.08 | | Crippen Method |
| logp | 5.928 | | Crippen Method |
| mcvol | 298.590 | ml/mol | McGowan Method |
| pc | 1485.00 | kPa | Joback Method |
| rinpol | 2785.00 | | NIST Webbook |
| rinpol | 2785.00 | | NIST Webbook |
| tb | 977.37 | K | Joback Method |
| tc | 1216.62 | K | Joback Method |
| tf | 635.93 | K | Joback Method |
| vc | 1.131 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 879.91 | J/mol×K | 977.37 | Joback Method |
| cpg | 891.37 | J/mol×K | 1017.24 | Joback Method |
| cpg | 901.54 | J/mol×K | 1057.12 | Joback Method |
| cpg | 910.50 | J/mol×K | 1096.99 | Joback Method |
| cpg | 918.30 | J/mol×K | 1136.87 | Joback Method |
| cpg | 925.00 | J/mol×K | 1176.74 | Joback Method |
| cpg | 930.65 | J/mol×K | 1216.62 | Joback Method |
| dvisc | 0.0001957 | Pa×s | 635.93 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001250 | Pa×s | 692.84 | Joback Method |
| dvisc | 0.0000855 | Pa×s | 749.74 | Joback Method |
| dvisc | 0.0000617 | Pa×s | 806.65 | Joback Method |
| dvisc | 0.0000465 | Pa×s | 863.56 | Joback Method |
| dvisc | 0.0000362 | Pa×s | 920.46 | Joback Method |
| dvisc | 0.0000291 | Pa×s | 977.37 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U369927&Units=SI |
| **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 |

# 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 |