# Diethylmalonic acid, 4-chloro-2-methylphenyl dodecyl ester

**Inchi:** InChI=1S/C26H41ClO4/c1-5-8-9-10-11-12-13-14-15-16-19-30-24(28)26(6-2,7-3)25(29)31

**InchiKey:** JOTXNXXMRNQLLA-UHFFFAOYSA-N

**Formula:** C26H41ClO4

**SMILES:** CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1C

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

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -215.74 | kJ/mol | Joback Method |
| hf | -880.47 | kJ/mol | Joback Method |
| hfus | 58.72 | kJ/mol | Joback Method |
| hvap | 98.47 | kJ/mol | Joback Method |
| log10ws | -8.68 | | Crippen Method |
| logp | 7.824 | | Crippen Method |
| mcvol | 380.560 | ml/mol | McGowan Method |
| pc | 896.95 | kPa | Joback Method |
| rinpol | 2974.00 | | NIST Webbook |
| rinpol | 2974.00 | | NIST Webbook |
| tb | 1017.70 | K | Joback Method |
| tc | 1246.25 | K | Joback Method |
| tf | 610.90 | K | Joback Method |
| vc | 1.470 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1268.95 | J/mol×K | 1017.70 | Joback Method |
| cpg | 1285.25 | J/mol×K | 1055.79 | Joback Method |
| cpg | 1300.09 | J/mol×K | 1093.88 | Joback Method |
| cpg | 1313.56 | J/mol×K | 1131.97 | Joback Method |
| cpg | 1325.72 | J/mol×K | 1170.06 | Joback Method |
| cpg | 1336.65 | J/mol×K | 1208.15 | Joback Method |
| cpg | 1346.43 | J/mol×K | 1246.25 | Joback Method |
| dvisc | 0.0001813 | Pa×s | 610.90 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000968 | Pa×s | 678.70 | Joback Method |
| dvisc | 0.0000579 | Pa×s | 746.50 | Joback Method |
| dvisc | 0.0000377 | Pa×s | 814.30 | Joback Method |
| dvisc | 0.0000263 | Pa×s | 882.10 | Joback Method |
| dvisc | 0.0000193 | Pa×s | 949.90 | Joback Method |
| dvisc | 0.0000147 | Pa×s | 1017.70 | 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=U370116&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 |