# Diethylmalonic acid, 2-chloro-5-methylphenyl undecyl ester

**Inchi:** InChI=1S/C25H39ClO4/c1-5-8-9-10-11-12-13-14-15-18-29-23(27)25(6-2,7-3)24(28)30-22

**InchiKey:** JMYBAAJYTVZPGS-UHFFFAOYSA-N

**Formula:** C25H39ClO4

**SMILES:** CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(C)ccc1Cl

**Mol. weight [g/mol]:** 439.03

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -224.16 | kJ/mol | Joback Method |
| hf | -859.83 | kJ/mol | Joback Method |
| hfus | 56.13 | kJ/mol | Joback Method |
| hvap | 96.24 | kJ/mol | Joback Method |
| log10ws | -8.26 | | Crippen Method |
| logp | 7.434 | | Crippen Method |
| mcvol | 366.470 | ml/mol | McGowan Method |
| pc | 950.84 | kPa | Joback Method |
| rinpol | 2831.00 | | NIST Webbook |
| rinpol | 2831.00 | | NIST Webbook |
| tb | 994.82 | K | Joback Method |
| tc | 1217.98 | K | Joback Method |
| tf | 599.63 | K | Joback Method |
| vc | 1.413 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1206.95 | J/mol×K | 994.82 | Joback Method |
| cpg | 1222.98 | J/mol×K | 1032.01 | Joback Method |
| cpg | 1237.62 | J/mol×K | 1069.21 | Joback Method |
| cpg | 1250.94 | J/mol×K | 1106.40 | Joback Method |
| cpg | 1263.02 | J/mol×K | 1143.59 | Joback Method |
| cpg | 1273.91 | J/mol×K | 1180.78 | Joback Method |
| cpg | 1283.68 | J/mol×K | 1217.98 | Joback Method |
| dvisc | 0.0002061 | Pa×s | 599.63 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001111 | Pa×s | 665.50 | Joback Method |
| dvisc | 0.0000670 | Pa×s | 731.36 | Joback Method |
| dvisc | 0.0000439 | Pa×s | 797.23 | Joback Method |
| dvisc | 0.0000307 | Pa×s | 863.09 | Joback Method |
| dvisc | 0.0000225 | Pa×s | 928.95 | Joback Method |
| dvisc | 0.0000173 | Pa×s | 994.82 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370460&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 |