# Diethylmalonic acid, 2,3-dichlorophenyl undecyl ester

**Inchi:** InChI=1S/C24H36Cl2O4/c1-4-7-8-9-10-11-12-13-14-18-29-22(27)24(5-2,6-3)23(28)30-20
**InchiKey:** BZWAGFBDASLUBF-UHFFFAOYSA-N
**Formula:** C24H36Cl2O4
**SMILES:** CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(Cl)c1Cl
**Mol. weight [g/mol]:** 459.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -244.51 | kJ/mol | Joback Method |
| hf | -854.93 | kJ/mol | Joback Method |
| hfus | 57.73 | kJ/mol | Joback Method |
| hvap | 98.40 | kJ/mol | Joback Method |
| log10ws | -8.47 | | Crippen Method |
| logp | 7.779 | | Crippen Method |
| mcvol | 364.620 | ml/mol | McGowan Method |
| pc | 986.40 | kPa | Joback Method |
| rinpol | 2922.00 | | NIST Webbook |
| rinpol | 2922.00 | | NIST Webbook |
| tb | 1009.37 | K | Joback Method |
| tc | 1235.86 | K | Joback Method |
| tf | 618.28 | K | Joback Method |
| vc | 1.407 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1169.80 | J/mol×K | 1009.37 | Joback Method |
| cpg | 1184.46 | J/mol×K | 1047.12 | Joback Method |
| cpg | 1197.79 | J/mol×K | 1084.87 | Joback Method |
| cpg | 1209.87 | J/mol×K | 1122.62 | Joback Method |
| cpg | 1220.75 | J/mol×K | 1160.37 | Joback Method |
| cpg | 1230.52 | J/mol×K | 1198.11 | Joback Method |
| cpg | 1239.24 | J/mol×K | 1235.86 | Joback Method |
| dvisc | 0.0001841 | Pa×s | 618.28 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001021 | Pa×s | 683.46 | Joback Method |
| dvisc | 0.0000628 | Pa×s | 748.64 | Joback Method |
| dvisc | 0.0000417 | Pa×s | 813.82 | Joback Method |
| dvisc | 0.0000294 | Pa×s | 879.01 | Joback Method |
| dvisc | 0.0000218 | Pa×s | 944.19 | Joback Method |
| dvisc | 0.0000168 | Pa×s | 1009.37 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370039&Units=SI |

# 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 |