# Diethylmalonic acid, 2,4-dichloronaphth-1-yl hexyl ester

**Inchi:** InChI=1S/C23H28Cl2O4/c1-4-7-8-11-14-28-21(26)23(5-2,6-3)22(27)29-20-17-13-10-9-12

**InchiKey:** KQBAYSSCGMGPQJ-UHFFFAOYSA-N

**Formula:** C23H28Cl2O4

**SMILES:** CCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)c2ccccc12

**Mol. weight [g/mol]:** 439.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -155.91 | kJ/mol | Joback Method |
| hf | -654.69 | kJ/mol | Joback Method |
| hfus | 51.77 | kJ/mol | Joback Method |
| hvap | 98.48 | kJ/mol | Joback Method |
| log10ws | -8.19 | | Crippen Method |
| logp | 6.982 | | Crippen Method |
| mcvol | 331.070 | ml/mol | McGowan Method |
| pc | 1224.27 | kPa | Joback Method |
| rinpol | 2993.00 | | NIST Webbook |
| rinpol | 2993.00 | | NIST Webbook |
| tb | 1010.45 | K | Joback Method |
| tc | 1242.21 | K | Joback Method |
| tf | 652.23 | K | Joback Method |
| vc | 1.272 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1024.26 | J/mol×K | 1010.45 | Joback Method |
| cpg | 1080.31 | J/mol×K | 1203.58 | Joback Method |
| cpg | 1070.77 | J/mol×K | 1164.96 | Joback Method |
| cpg | 1060.48 | J/mol×K | 1126.33 | Joback Method |
| cpg | 1049.36 | J/mol×K | 1087.70 | Joback Method |
| cpg | 1037.32 | J/mol×K | 1049.08 | Joback Method |
| cpg | 1089.19 | J/mol×K | 1242.21 | Joback Method |
| dvisc | 0.0000425 | Pa×s | 1010.45 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000524 | Pa×s | 950.75 | Joback Method |
| dvisc | 0.0000665 | Pa×s | 891.04 | Joback Method |
| dvisc | 0.0000873 | Pa×s | 831.34 | Joback Method |
| dvisc | 0.0001195 | Pa×s | 771.64 | Joback Method |
| dvisc | 0.0001725 | Pa×s | 711.93 | Joback Method |
| dvisc | 0.0002664 | Pa×s | 652.23 | 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=U370054&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 |