# Diethylmalonic acid, pentadecyl phenethyl ester

**Inchi:** InChI=1S/C30H50O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-21-25-33-28(31)30(5-2,6-3)29

**InchiKey:** PIWMDNSIGNHWIH-UHFFFAOYSA-N

**Formula:** C30H50O4

**SMILES:** CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCc1ccccc1

**Mol. weight [g/mol]:** 474.72

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -150.87 | kJ/mol | Joback Method |
| hf | -924.35 | kJ/mol | Joback Method |
| hfus | 65.66 | kJ/mol | Joback Method |
| hvap | 101.67 | kJ/mol | Joback Method |
| log10ws | -8.97 | | Crippen Method |
| logp | 8.213 | | Crippen Method |
| mcvol | 424.680 | ml/mol | McGowan Method |
| pc | 748.15 | kPa | Joback Method |
| rinpol | 3163.00 | | NIST Webbook |
| tb | 1061.83 | K | Joback Method |
| tc | 1308.19 | K | Joback Method |
| tf | 601.02 | K | Joback Method |
| vc | 1.645 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1497.51 | J/mol×K | 1061.83 | Joback Method |
| cpg | 1577.81 | J/mol×K | 1267.13 | Joback Method |
| cpg | 1564.65 | J/mol×K | 1226.07 | Joback Method |
| cpg | 1550.17 | J/mol×K | 1185.01 | Joback Method |
| cpg | 1534.24 | J/mol×K | 1143.95 | Joback Method |
| cpg | 1516.73 | J/mol×K | 1102.89 | Joback Method |
| cpg | 1589.78 | J/mol×K | 1308.19 | Joback Method |
| dvisc | 0.0000088 | Pa×s | 1061.83 | Joback Method |
| dvisc | 0.0000120 | Pa×s | 985.03 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000171 | Pa×s | 908.23 | Joback Method |
| dvisc | 0.0000261 | Pa×s | 831.42 | Joback Method |
| dvisc | 0.0000433 | Pa×s | 754.62 | Joback Method |
| dvisc | 0.0000807 | Pa×s | 677.82 | Joback Method |
| dvisc | 0.0001763 | Pa×s | 601.02 | Joback Method |

# Sources

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|---|---|
| **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=U369558&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 |