# Diethylmalonic acid, 4-acetylphenyl pentadecyl ester

**Inchi:** InChI=1S/C30H48O5/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-24-34-28(32)30(6-2,7-3)2

**InchiKey:** OLFPWWNGPWNROU-UHFFFAOYSA-N

**Formula:** C30H48O5

**SMILES:** CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(C(C)=O)cc1

**Mol. weight [g/mol]:** 488.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -289.42 | kJ/mol | Joback Method |
| hf | -1048.40 | kJ/mol | Joback Method |
| hfus | 66.87 | kJ/mol | Joback Method |
| hvap | 109.07 | kJ/mol | Joback Method |
| log10ws | -9.44 | | Crippen Method |
| logp | 8.235 | | Crippen Method |
| mcvol | 426.250 | ml/mol | McGowan Method |
| pc | 768.19 | kPa | Joback Method |
| rinpol | 3413.00 | | NIST Webbook |
| tb | 1120.68 | K | Joback Method |
| tc | 1386.39 | K | Joback Method |
| tf | 663.47 | K | Joback Method |
| vc | 1.651 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1508.05 | J/mol×K | 1120.68 | Joback Method |
| cpg | 1525.03 | J/mol×K | 1164.97 | Joback Method |
| cpg | 1540.12 | J/mol×K | 1209.25 | Joback Method |
| cpg | 1553.46 | J/mol×K | 1253.54 | Joback Method |
| cpg | 1565.21 | J/mol×K | 1297.82 | Joback Method |
| cpg | 1575.51 | J/mol×K | 1342.11 | Joback Method |
| cpg | 1584.50 | J/mol×K | 1386.39 | Joback Method |
| dvisc | 0.0001201 | Pa×s | 663.47 | Joback Method |
| dvisc | 0.0000612 | Pa×s | 739.67 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000354 | Pa×s | 815.87 | Joback Method |
| dvisc | 0.0000225 | Pa×s | 892.07 | Joback Method |
| dvisc | 0.0000153 | Pa×s | 968.28 | Joback Method |
| dvisc | 0.0000110 | Pa×s | 1044.48 | Joback Method |
| dvisc | 0.0000083 | Pa×s | 1120.68 | Joback Method |

# Sources

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|---|---|
| **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=U370093&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 |