# Diethylmalonic acid, 2-ethylphenyl tetradecyl ester

**Inchi:** InChI=1S/C29H48O4/c1-5-9-10-11-12-13-14-15-16-17-18-21-24-32-27(30)29(7-3,8-4)28

**InchiKey:** YUKUTPCWHJPNPL-UHFFFAOYSA-N

**Formula:** C29H48O4

**SMILES:** CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1CC

**Mol. weight [g/mol]:** 460.69

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -168.92 | kJ/mol | Joback Method |
| hf | -915.18 | kJ/mol | Joback Method |
| hfus | 62.68 | kJ/mol | Joback Method |
| hvap | 100.10 | kJ/mol | Joback Method |
| log10ws | -9.16 | | Crippen Method |
| logp | 8.205 | | Crippen Method |
| mcvol | 410.590 | ml/mol | McGowan Method |
| pc | 782.43 | kPa | Joback Method |
| rinpol | 3025.00 | | NIST Webbook |
| tb | 1043.93 | K | Joback Method |
| tc | 1282.64 | K | Joback Method |
| tf | 602.27 | K | Joback Method |
| vc | 1.589 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1432.98 | J/mol×K | 1043.93 | Joback Method |
| cpg | 1510.33 | J/mol×K | 1242.86 | Joback Method |
| cpg | 1497.76 | J/mol×K | 1203.07 | Joback Method |
| cpg | 1483.84 | J/mol×K | 1163.29 | Joback Method |
| cpg | 1468.47 | J/mol×K | 1123.50 | Joback Method |
| cpg | 1451.55 | J/mol×K | 1083.72 | Joback Method |
| cpg | 1521.67 | J/mol×K | 1282.64 | Joback Method |
| dvisc | 0.0000107 | Pa×s | 1043.93 | Joback Method |
| dvisc | 0.0000143 | Pa×s | 970.32 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000201 | Pa×s | 896.71 | Joback Method |
| dvisc | 0.0000299 | Pa×s | 823.10 | Joback Method |
| dvisc | 0.0000482 | Pa×s | 749.49 | Joback Method |
| dvisc | 0.0000861 | Pa×s | 675.88 | Joback Method |
| dvisc | 0.0001776 | Pa×s | 602.27 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370253&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 |