# Diethylmalonic acid, 3-methylbutyl tetradecyl ester

**Inchi:** InChI=1S/C26H50O4/c1-6-9-10-11-12-13-14-15-16-17-18-19-21-29-24(27)26(7-2,8-3)25

**InchiKey:** FOTWYFMFCBLLRB-UHFFFAOYSA-N

**Formula:** C26H50O4

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

**Mol. weight [g/mol]:** 426.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -299.40 | kJ/mol | Joback Method |
| hf | -1083.60 | kJ/mol | Joback Method |
| hfus | 57.73 | kJ/mol | Joback Method |
| hvap | 90.10 | kJ/mol | Joback Method |
| log10ws | -7.95 | | Crippen Method |
| logp | 7.626 | | Crippen Method |
| mcvol | 392.080 | ml/mol | McGowan Method |
| pc | 773.75 | kPa | Joback Method |
| rinpol | 2627.00 | | NIST Webbook |
| rinpol | 2627.00 | | NIST Webbook |
| tb | 943.19 | K | Joback Method |
| tc | 1157.23 | K | Joback Method |
| tf | 514.52 | K | Joback Method |
| vc | 1.522 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1345.34 | J/mol×K | 943.19 | Joback Method |
| cpg | 1366.13 | J/mol×K | 978.86 | Joback Method |
| cpg | 1385.41 | J/mol×K | 1014.54 | Joback Method |
| cpg | 1403.24 | J/mol×K | 1050.21 | Joback Method |
| cpg | 1419.69 | J/mol×K | 1085.88 | Joback Method |
| cpg | 1434.82 | J/mol×K | 1121.56 | Joback Method |
| cpg | 1448.69 | J/mol×K | 1157.23 | Joback Method |
| dvisc | 0.0004231 | Pa×s | 514.52 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001730 | Pa×s | 585.97 | Joback Method |
| dvisc | 0.0000859 | Pa×s | 657.41 | Joback Method |
| dvisc | 0.0000490 | Pa×s | 728.86 | Joback Method |
| dvisc | 0.0000308 | Pa×s | 800.30 | Joback Method |
| dvisc | 0.0000210 | Pa×s | 871.75 | Joback Method |
| dvisc | 0.0000151 | Pa×s | 943.19 | Joback Method |

# Sources

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|---|---|
| **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=U369393&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |