# Diethylmalonic acid, 2-methoxyethyl pentadecyl ester

**Inchi:** InChI=1S/C25H48O5/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-29-23(26)25(6-2,7-3)2

**InchiKey:** LERXEBBODFOSDM-UHFFFAOYSA-N

**Formula:** C25H48O5

**SMILES:** CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCOC

**Mol. weight [g/mol]:** 428.65

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -410.38 | kJ/mol | Joback Method |
| hf | -1189.90 | kJ/mol | Joback Method |
| hfus | 59.85 | kJ/mol | Joback Method |
| hvap | 90.67 | kJ/mol | Joback Method |
| log10ws | -6.86 | | Crippen Method |
| logp | 6.617 | | Crippen Method |
| mcvol | 383.860 | ml/mol | McGowan Method |
| pc | 805.25 | kPa | Joback Method |
| rinpol | 2713.00 | | NIST Webbook |
| rinpol | 2713.00 | | NIST Webbook |
| tb | 943.17 | K | Joback Method |
| tc | 1157.86 | K | Joback Method |
| tf | 540.48 | K | Joback Method |
| vc | 1.490 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1313.06 | J/mol×K | 943.17 | Joback Method |
| cpg | 1397.72 | J/mol×K | 1122.08 | Joback Method |
| cpg | 1383.78 | J/mol×K | 1086.30 | Joback Method |
| cpg | 1368.39 | J/mol×K | 1050.52 | Joback Method |
| cpg | 1351.51 | J/mol×K | 1014.73 | Joback Method |
| cpg | 1333.08 | J/mol×K | 978.95 | Joback Method |
| cpg | 1410.26 | J/mol×K | 1157.86 | Joback Method |
| dvisc | 0.0000142 | Pa×s | 943.17 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000193 | Pa×s | 876.06 | Joback Method |
| dvisc | 0.0000276 | Pa×s | 808.94 | Joback Method |
| dvisc | 0.0000420 | Pa×s | 741.83 | Joback Method |
| dvisc | 0.0000696 | Pa×s | 674.71 | Joback Method |
| dvisc | 0.0001290 | Pa×s | 607.60 | Joback Method |
| dvisc | 0.0002783 | Pa×s | 540.48 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370682&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 |

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