# Diethylmalonic acid, dodecyl heptyl ester

**Inchi:** InChI=1S/C26H50O4/c1-5-9-11-13-14-15-16-17-19-21-23-30-25(28)26(7-3,8-4)24(27)29-
**InchiKey:** ITWRRYFNZDTQST-UHFFFAOYSA-N
**Formula:** C26H50O4
**SMILES:** CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCC
**Mol. weight [g/mol]:** 426.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -296.96 | kJ/mol | Joback Method |
| hf | -1078.32 | kJ/mol | Joback Method |
| hfus | 61.26 | kJ/mol | Joback Method |
| hvap | 90.49 | kJ/mol | Joback Method |
| log10ws | -8.19 | | Crippen Method |
| logp | 7.771 | | Crippen Method |
| mcvol | 392.080 | ml/mol | McGowan Method |
| pc | 770.32 | kPa | Joback Method |
| rinpol | 2651.00 | | NIST Webbook |
| tb | 943.63 | K | Joback Method |
| tc | 1158.72 | K | Joback Method |
| tf | 529.52 | K | Joback Method |
| vc | 1.528 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1344.97 | J/mol×K | 943.63 | Joback Method |
| cpg | 1365.90 | J/mol×K | 979.48 | Joback Method |
| cpg | 1385.32 | J/mol×K | 1015.33 | Joback Method |
| cpg | 1403.28 | J/mol×K | 1051.17 | Joback Method |
| cpg | 1419.86 | J/mol×K | 1087.02 | Joback Method |
| cpg | 1435.13 | J/mol×K | 1122.87 | Joback Method |
| cpg | 1449.14 | J/mol×K | 1158.72 | Joback Method |
| dvisc | 0.0003659 | Pa×s | 529.52 | Joback Method |
| dvisc | 0.0001622 | Pa×s | 598.54 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000851 | Pa×s | 667.56 | Joback Method |
| dvisc | 0.0000504 | Pa×s | 736.58 | Joback Method |
| dvisc | 0.0000326 | Pa×s | 805.59 | Joback Method |
| dvisc | 0.0000226 | Pa×s | 874.61 | Joback Method |
| dvisc | 0.0000166 | Pa×s | 943.63 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U369520&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 |

# 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 |