# Diethylmalonic acid, 3,7-dimethyloctyl tetradecyl ester

**Inchi:** InChI=1S/C31H60O4/c1-7-10-11-12-13-14-15-16-17-18-19-20-25-34-29(32)31(8-2,9-3)3
**InchiKey:** ABGPBEHBSBTUBP-UHFFFAOYSA-N
**Formula:** C31H60O4
**SMILES:** CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCCC(C)C
**Mol. weight [g/mol]:** 496.81

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -259.74 | kJ/mol | Joback Method |
| hf | -1192.08 | kJ/mol | Joback Method |
| hfus | 67.16 | kJ/mol | Joback Method |
| hvap | 100.84 | kJ/mol | Joback Method |
| log10ws | -9.80 | | Crippen Method |
| logp | 9.433 | | Crippen Method |
| mcvol | 462.530 | ml/mol | McGowan Method |
| pc | 604.58 | kPa | Joback Method |
| rinpol | 3020.00 | | NIST Webbook |
| rinpol | 3020.00 | | NIST Webbook |
| tb | 1057.15 | K | Joback Method |
| tc | 1321.25 | K | Joback Method |
| tf | 555.87 | K | Joback Method |
| vc | 1.796 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1670.88 | J/mol×K | 1057.15 | Joback Method |
| cpg | 1694.76 | J/mol×K | 1101.17 | Joback Method |
| cpg | 1716.36 | J/mol×K | 1145.18 | Joback Method |
| cpg | 1735.83 | J/mol×K | 1189.20 | Joback Method |
| cpg | 1753.35 | J/mol×K | 1233.22 | Joback Method |
| cpg | 1769.04 | J/mol×K | 1277.23 | Joback Method |
| cpg | 1783.08 | J/mol×K | 1321.25 | Joback Method |
| dvisc | 0.0002305 | Pa×s | 555.87 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000842 | Pa×s | 639.42 | Joback Method |
| dvisc | 0.0000389 | Pa×s | 722.96 | Joback Method |
| dvisc | 0.0000210 | Pa×s | 806.51 | Joback Method |
| dvisc | 0.0000128 | Pa×s | 890.06 | Joback Method |
| dvisc | 0.0000085 | Pa×s | 973.60 | Joback Method |
| dvisc | 0.0000060 | Pa×s | 1057.15 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U369413&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

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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 |