# Dimethylmalonic acid, 3-phenylpropyl tridecyl ester

**Inchi:** InChI=1S/C27H44O4/c1-4-5-6-7-8-9-10-11-12-13-17-22-30-25(28)27(2,3)26(29)31-23-18
**InchiKey:** QYCUHUBRYOEMAF-UHFFFAOYSA-N
**Formula:** C27H44O4
**SMILES:** CCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCc1ccccc1
**Mol. weight [g/mol]:** 432.64

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -176.13 | kJ/mol | Joback Method |
| hf | -862.43 | kJ/mol | Joback Method |
| hfus | 57.89 | kJ/mol | Joback Method |
| hvap | 94.99 | kJ/mol | Joback Method |
| log10ws | -7.71 | | Crippen Method |
| logp | 7.043 | | Crippen Method |
| mcvol | 382.410 | ml/mol | McGowan Method |
| pc | 881.57 | kPa | Joback Method |
| rinpol | 2927.00 | | NIST Webbook |
| tb | 993.19 | K | Joback Method |
| tc | 1216.27 | K | Joback Method |
| tf | 567.21 | K | Joback Method |
| vc | 1.476 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1306.86 | J/mol×K | 993.19 | Joback Method |
| cpg | 1324.82 | J/mol×K | 1030.37 | Joback Method |
| cpg | 1341.33 | J/mol×K | 1067.55 | Joback Method |
| cpg | 1356.47 | J/mol×K | 1104.73 | Joback Method |
| cpg | 1370.34 | J/mol×K | 1141.91 | Joback Method |
| cpg | 1383.02 | J/mol×K | 1179.09 | Joback Method |
| cpg | 1394.60 | J/mol×K | 1216.27 | Joback Method |
| dvisc | 0.0002676 | Pa×s | 567.21 | Joback Method |
| dvisc | 0.0001254 | Pa×s | 638.21 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000684 | Pa×s | 709.20 | Joback Method |
| dvisc | 0.0000417 | Pa×s | 780.20 | Joback Method |
| dvisc | 0.0000276 | Pa×s | 851.20 | Joback Method |
| dvisc | 0.0000194 | Pa×s | 922.19 | Joback Method |
| dvisc | 0.0000144 | Pa×s | 993.19 | 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=U361842&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 |