# Dimethylmalonic acid, di(3-phenylpropyl) ester

**Inchi:** InChI=1S/C23H28O4/c1-23(2,21(24)26-17-9-15-19-11-5-3-6-12-19)22(25)27-18-10-16-2
**InchiKey:** NYJIXRFZLWGUNS-UHFFFAOYSA-N
**Formula:** C23H28O4
**SMILES:** CC(C)(C(=O)OCCCc1ccccc1)C(=O)OCCCc1ccccc1
**Mol. weight [g/mol]:** 368.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -97.40 | kJ/mol | Joback Method |
| hf | -543.34 | kJ/mol | Joback Method |
| hfus | 41.57 | kJ/mol | Joback Method |
| hvap | 88.36 | kJ/mol | Joback Method |
| log10ws | -5.14 | | Crippen Method |
| logp | 4.365 | | Crippen Method |
| mcvol | 302.290 | ml/mol | McGowan Method |
| pc | 1420.78 | kPa | Joback Method |
| rinpol | 2694.00 | | NIST Webbook |
| tb | 928.35 | K | Joback Method |
| tc | 1154.94 | K | Joback Method |
| tf | 548.55 | K | Joback Method |
| vc | 1.145 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 958.49 | J/mol×K | 928.35 | Joback Method |
| cpg | 973.24 | J/mol×K | 966.11 | Joback Method |
| cpg | 986.70 | J/mol×K | 1003.88 | Joback Method |
| cpg | 998.94 | J/mol×K | 1041.64 | Joback Method |
| cpg | 1010.05 | J/mol×K | 1079.41 | Joback Method |
| cpg | 1020.11 | J/mol×K | 1117.17 | Joback Method |
| cpg | 1029.21 | J/mol×K | 1154.94 | Joback Method |
| dvisc | 0.0003826 | Pa×s | 548.55 | Joback Method |
| dvisc | 0.0001970 | Pa×s | 611.85 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001148 | Pa×s | 675.15 | Joback Method |
| dvisc | 0.0000735 | Pa×s | 738.45 | Joback Method |
| dvisc | 0.0000504 | Pa×s | 801.75 | Joback Method |
| dvisc | 0.0000366 | Pa×s | 865.05 | Joback Method |
| dvisc | 0.0000277 | Pa×s | 928.35 | Joback Method |

# Sources

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|---|---|
| **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=U361847&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |