# Dimethylmalonic acid, 2-naphthylmethyl pentyl ester

**Inchi:** InChI=1S/C21H26O4/c1-4-5-8-13-24-19(22)21(2,3)20(23)25-15-16-11-12-17-9-6-7-10-18

**InchiKey:** CCAJMQZZWYCLHR-UHFFFAOYSA-N

**Formula:** C21H26O4

**SMILES:** CCCCCOC(=O)C(C)(C)C(=O)OCc1ccc2ccccc2c1

**Mol. weight [g/mol]:** 342.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -129.63 | kJ/mol | Joback Method |
| hf | -558.99 | kJ/mol | Joback Method |
| hfus | 38.98 | kJ/mol | Joback Method |
| hvap | 83.93 | kJ/mol | Joback Method |
| log10ws | -5.82 | | Crippen Method |
| logp | 4.643 | | Crippen Method |
| mcvol | 278.410 | ml/mol | McGowan Method |
| pc | 1523.50 | kPa | Joback Method |
| rinpol | 2551.00 | | NIST Webbook |
| rinpol | 2551.00 | | NIST Webbook |
| tb | 879.87 | K | Joback Method |
| tc | 1099.65 | K | Joback Method |
| tf | 544.81 | K | Joback Method |
| vc | 1.062 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 861.88 | J/mol×K | 879.87 | Joback Method |
| cpg | 926.43 | J/mol×K | 1063.02 | Joback Method |
| cpg | 915.38 | J/mol×K | 1026.39 | Joback Method |
| cpg | 903.48 | J/mol×K | 989.76 | Joback Method |
| cpg | 890.65 | J/mol×K | 953.13 | Joback Method |
| cpg | 876.81 | J/mol×K | 916.50 | Joback Method |
| cpg | 936.71 | J/mol×K | 1099.65 | Joback Method |
| dvisc | 0.0000742 | Pa×s | 879.87 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000931 | Pa×s | 824.03 | Joback Method |
| dvisc | 0.0001208 | Pa×s | 768.18 | Joback Method |
| dvisc | 0.0001632 | Pa×s | 712.34 | Joback Method |
| dvisc | 0.0002321 | Pa×s | 656.50 | Joback Method |
| dvisc | 0.0003525 | Pa×s | 600.65 | Joback Method |
| dvisc | 0.0005831 | Pa×s | 544.81 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U363858&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 |