# Diethylmalonic acid, 2,3-dimethylphenyl pentyl ester

**Inchi:** InChI=1S/C20H30O4/c1-6-9-10-14-23-18(21)20(7-2,8-3)19(22)24-17-13-11-12-15(4)16(1

**InchiKey:** ZQWGZGAITSDFNS-UHFFFAOYSA-N

**Formula:** C20H30O4

**SMILES:** CCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1C

**Mol. weight [g/mol]:** 334.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -254.33 | kJ/mol | Joback Method |
| hf | -740.89 | kJ/mol | Joback Method |
| hfus | 38.98 | kJ/mol | Joback Method |
| hvap | 80.73 | kJ/mol | Joback Method |
| log10ws | -5.54 | | Crippen Method |
| logp | 4.749 | | Crippen Method |
| mcvol | 283.780 | ml/mol | McGowan Method |
| pc | 1345.70 | kPa | Joback Method |
| rinpol | 2202.00 | | NIST Webbook |
| rinpol | 2202.00 | | NIST Webbook |
| tb | 842.99 | K | Joback Method |
| tc | 1048.98 | K | Joback Method |
| tf | 513.36 | K | Joback Method |
| vc | 1.085 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 878.07 | J/mol×K | 842.99 | Joback Method |
| cpg | 894.28 | J/mol×K | 877.32 | Joback Method |
| cpg | 909.34 | J/mol×K | 911.65 | Joback Method |
| cpg | 923.28 | J/mol×K | 945.99 | Joback Method |
| cpg | 936.14 | J/mol×K | 980.32 | Joback Method |
| cpg | 947.97 | J/mol×K | 1014.65 | Joback Method |
| cpg | 958.78 | J/mol×K | 1048.98 | Joback Method |
| dvisc | 0.0004658 | Pa×s | 513.36 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002598 | Pa×s | 568.30 | Joback Method |
| dvisc | 0.0001606 | Pa×s | 623.24 | Joback Method |
| dvisc | 0.0001073 | Pa×s | 678.17 | Joback Method |
| dvisc | 0.0000762 | Pa×s | 733.11 | Joback Method |
| dvisc | 0.0000567 | Pa×s | 788.05 | Joback Method |
| dvisc | 0.0000439 | Pa×s | 842.99 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370566&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 |