# Diethylmalonic acid, di(5-methylhex-2-yl) ester

**Inchi:** InChI=1S/C21H40O4/c1-9-21(10-2,19(22)24-17(7)13-11-15(3)4)20(23)25-18(8)14-12-16
**InchiKey:** NUYNZFWIBSLNPK-UHFFFAOYSA-N
**Formula:** C21H40O4
**SMILES:** CCC(CC)(C(=O)OC(C)CCC(C)C)C(=O)OC(C)CCC(C)C
**Mol. weight [g/mol]:** 356.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -348.82 | kJ/mol | Joback Method |
| hf | -996.24 | kJ/mol | Joback Method |
| hfus | 34.21 | kJ/mol | Joback Method |
| hvap | 77.80 | kJ/mol | Joback Method |
| log10ws | -5.84 | | Crippen Method |
| logp | 5.529 | | Crippen Method |
| mcvol | 321.630 | ml/mol | McGowan Method |
| pc | 1046.65 | kPa | Joback Method |
| rinpol | 1964.00 | | NIST Webbook |
| tb | 827.47 | K | Joback Method |
| tc | 1019.97 | K | Joback Method |
| tf | 413.17 | K | Joback Method |
| vc | 1.224 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1032.90 | J/mol×K | 827.47 | Joback Method |
| cpg | 1051.87 | J/mol×K | 859.55 | Joback Method |
| cpg | 1069.65 | J/mol×K | 891.64 | Joback Method |
| cpg | 1086.28 | J/mol×K | 923.72 | Joback Method |
| cpg | 1101.79 | J/mol×K | 955.80 | Joback Method |
| cpg | 1116.22 | J/mol×K | 987.88 | Joback Method |
| cpg | 1129.61 | J/mol×K | 1019.97 | Joback Method |
| dvisc | 0.0016281 | Pa×s | 413.17 | Joback Method |
| dvisc | 0.0004983 | Pa×s | 482.22 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002052 | Pa×s | 551.27 | Joback Method |
| dvisc | 0.0001029 | Pa×s | 620.32 | Joback Method |
| dvisc | 0.0000593 | Pa×s | 689.37 | Joback Method |
| dvisc | 0.0000378 | Pa×s | 758.42 | Joback Method |
| dvisc | 0.0000259 | Pa×s | 827.47 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U369301&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