# Diethylmalonic acid, ethyl 5-methoxy-3-methylpentyl ester

**Inchi:** InChI=1S/C16H30O5/c1-6-16(7-2,14(17)20-8-3)15(18)21-12-10-13(4)9-11-19-5/h13H,6-1

**InchiKey:** XDDCUMCCWBDLAW-UHFFFAOYSA-N

**Formula:** C16H30O5

**SMILES:** CCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCOC

**Mol. weight [g/mol]:** 302.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -488.60 | kJ/mol | Joback Method |
| hf | -1009.42 | kJ/mol | Joback Method |
| hfus | 33.02 | kJ/mol | Joback Method |
| hvap | 70.25 | kJ/mol | Joback Method |
| log10ws | -2.85 | | Crippen Method |
| logp | 2.962 | | Crippen Method |
| mcvol | 257.050 | ml/mol | McGowan Method |
| pc | 1421.85 | kPa | Joback Method |
| rinpol | 1787.00 | | NIST Webbook |
| tb | 736.81 | K | Joback Method |
| tc | 921.18 | K | Joback Method |
| tf | 424.05 | K | Joback Method |
| vc | 0.981 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 766.03 | J/mol×K | 736.81 | Joback Method |
| cpg | 782.81 | J/mol×K | 767.54 | Joback Method |
| cpg | 798.65 | J/mol×K | 798.27 | Joback Method |
| cpg | 813.57 | J/mol×K | 829.00 | Joback Method |
| cpg | 827.59 | J/mol×K | 859.72 | Joback Method |
| cpg | 840.70 | J/mol×K | 890.45 | Joback Method |
| cpg | 852.93 | J/mol×K | 921.18 | Joback Method |
| dvisc | 0.0010322 | Pa×s | 424.05 | Joback Method |
| dvisc | 0.0004815 | Pa×s | 476.18 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002611 | Pa×s | 528.30 | Joback Method |
| dvisc | 0.0001580 | Pa×s | 580.43 | Joback Method |
| dvisc | 0.0001039 | Pa×s | 632.56 | Joback Method |
| dvisc | 0.0000728 | Pa×s | 684.68 | Joback Method |
| dvisc | 0.0000537 | Pa×s | 736.81 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370761&Units=SI |

# 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 |