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

**Inchi:** InChI=1S/C14H25ClO4/c1-5-14(6-2,12(15)16)13(17)19-10-8-11(3)7-9-18-4/h11H,5-10H2

**InchiKey:** MHCZQIUCZJLRRW-UHFFFAOYSA-N

**Formula:** C14H25ClO4

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

**Mol. weight [g/mol]:** 292.80

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -412.37 | kJ/mol | Joback Method |
| hf | -851.66 | kJ/mol | Joback Method |
| hfus | 30.85 | kJ/mol | Joback Method |
| hvap | 67.77 | kJ/mol | Joback Method |
| log10ws | -3.08 | | Crippen Method |
| logp | 3.164 | | Crippen Method |
| mcvol | 235.240 | ml/mol | McGowan Method |
| pc | 1625.91 | kPa | Joback Method |
| rinpol | 1712.00 | | NIST Webbook |
| rinpol | 1712.00 | | NIST Webbook |
| tb | 706.06 | K | Joback Method |
| tc | 895.93 | K | Joback Method |
| tf | 409.20 | K | Joback Method |
| vc | 0.899 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 655.57 | J/mol×K | 706.06 | Joback Method |
| cpg | 724.01 | J/mol×K | 864.28 | Joback Method |
| cpg | 711.98 | J/mol×K | 832.64 | Joback Method |
| cpg | 699.14 | J/mol×K | 800.99 | Joback Method |
| cpg | 685.48 | J/mol×K | 769.35 | Joback Method |
| cpg | 670.96 | J/mol×K | 737.70 | Joback Method |
| cpg | 735.25 | J/mol×K | 895.93 | Joback Method |
| dvisc | 0.0000829 | Pa×s | 706.06 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001120 | Pa×s | 656.58 | Joback Method |
| dvisc | 0.0001588 | Pa×s | 607.11 | Joback Method |
| dvisc | 0.0002396 | Pa×s | 557.63 | Joback Method |
| dvisc | 0.0003917 | Pa×s | 508.15 | Joback Method |
| dvisc | 0.0007120 | Pa×s | 458.68 | Joback Method |
| dvisc | 0.0014953 | Pa×s | 409.20 | 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=U370774&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 |