# Diethylmalonic acid, 5-methylhex-2-yl octyl ester

**Inchi:** InChI=1S/C22H42O4/c1-7-10-11-12-13-14-17-25-20(23)22(8-2,9-3)21(24)26-19(6)16-15-
**InchiKey:** IBAQSTMIACDGCT-UHFFFAOYSA-N
**Formula:** C22H42O4
**SMILES:** CCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)CCC(C)C
**Mol. weight [g/mol]:** 370.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -335.52 | kJ/mol | Joback Method |
| hf | -1006.32 | kJ/mol | Joback Method |
| hfus | 43.85 | kJ/mol | Joback Method |
| hvap | 80.81 | kJ/mol | Joback Method |
| log10ws | -6.39 | | Crippen Method |
| logp | 6.064 | | Crippen Method |
| mcvol | 335.720 | ml/mol | McGowan Method |
| pc | 974.73 | kPa | Joback Method |
| rinpol | 2175.00 | | NIST Webbook |
| tb | 851.23 | K | Joback Method |
| tc | 1044.28 | K | Joback Method |
| tf | 454.44 | K | Joback Method |
| vc | 1.292 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1093.48 | J/mol×K | 851.23 | Joback Method |
| cpg | 1112.55 | J/mol×K | 883.41 | Joback Method |
| cpg | 1130.42 | J/mol×K | 915.58 | Joback Method |
| cpg | 1147.14 | J/mol×K | 947.76 | Joback Method |
| cpg | 1162.73 | J/mol×K | 979.93 | Joback Method |
| cpg | 1177.25 | J/mol×K | 1012.11 | Joback Method |
| cpg | 1190.72 | J/mol×K | 1044.28 | Joback Method |
| dvisc | 0.0008913 | Pa×s | 454.44 | Joback Method |
| dvisc | 0.0003412 | Pa×s | 520.57 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001622 | Pa×s | 586.70 | Joback Method |
| dvisc | 0.0000896 | Pa×s | 652.84 | Joback Method |
| dvisc | 0.0000552 | Pa×s | 718.97 | Joback Method |
| dvisc | 0.0000369 | Pa×s | 785.10 | Joback Method |
| dvisc | 0.0000263 | Pa×s | 851.23 | 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=U369300&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 |