# Diethylmalonic acid, 4-chloro-2-methylphenyl octyl ester

**Inchi:** InChI=1S/C22H33ClO4/c1-5-8-9-10-11-12-15-26-20(24)22(6-2,7-3)21(25)27-19-14-13-18

**InchiKey:** FOTBYQFMBZSIEI-UHFFFAOYSA-N

**Formula:** C22H33ClO4

**SMILES:** CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1C

**Mol. weight [g/mol]:** 396.95

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -249.42 | kJ/mol | Joback Method |
| hf | -797.91 | kJ/mol | Joback Method |
| hfus | 48.36 | kJ/mol | Joback Method |
| hvap | 89.57 | kJ/mol | Joback Method |
| log10ws | -7.01 | | Crippen Method |
| logp | 6.264 | | Crippen Method |
| mcvol | 324.200 | ml/mol | McGowan Method |
| pc | 1145.21 | kPa | Joback Method |
| rinpol | 2554.00 | | NIST Webbook |
| tb | 926.18 | K | Joback Method |
| tc | 1139.21 | K | Joback Method |
| tf | 565.82 | K | Joback Method |
| vc | 1.246 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1023.93 | J/mol×K | 926.18 | Joback Method |
| cpg | 1039.29 | J/mol×K | 961.69 | Joback Method |
| cpg | 1053.43 | J/mol×K | 997.19 | Joback Method |
| cpg | 1066.40 | J/mol×K | 1032.70 | Joback Method |
| cpg | 1078.24 | J/mol×K | 1068.20 | Joback Method |
| cpg | 1089.00 | J/mol×K | 1103.71 | Joback Method |
| cpg | 1098.73 | J/mol×K | 1139.21 | Joback Method |
| dvisc | 0.0002985 | Pa×s | 565.82 | Joback Method |
| dvisc | 0.0001659 | Pa×s | 625.88 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001022 | Pa×s | 685.94 | Joback Method |
| dvisc | 0.0000681 | Pa×s | 746.00 | Joback Method |
| dvisc | 0.0000482 | Pa×s | 806.06 | Joback Method |
| dvisc | 0.0000358 | Pa×s | 866.12 | Joback Method |
| dvisc | 0.0000276 | Pa×s | 926.18 | Joback Method |

# Sources

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|---|---|
| **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=U370112&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |