# Diethylmalonic acid, monochloride, 2,4-dichloro-6-formylphenyl ester

**Inchi:** InChI=1S/C14H13Cl3O4/c1-3-14(4-2,12(17)19)13(20)21-11-8(7-18)5-9(15)6-10(11)16/h5

**InchiKey:** NJWAUZQHFDLNDW-UHFFFAOYSA-N

**Formula:** C14H13Cl3O4

**SMILES:** CCC(CC)(C(=O)Cl)C(=O)Oc1c(Cl)cc(Cl)cc1C=O

**Mol. weight [g/mol]:** 351.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -344.79 | kJ/mol | Joback Method |
| hf | -629.10 | kJ/mol | Joback Method |
| hfus | 36.74 | kJ/mol | Joback Method |
| hvap | 85.50 | kJ/mol | Joback Method |
| log10ws | -5.18 | | Crippen Method |
| logp | 4.283 | | Crippen Method |
| mcvol | 231.660 | ml/mol | McGowan Method |
| pc | 2094.58 | kPa | Joback Method |
| rinpol | 2198.00 | | NIST Webbook |
| rinpol | 2198.00 | | NIST Webbook |
| tb | 849.22 | K | Joback Method |
| tc | 1079.70 | K | Joback Method |
| tf | 567.79 | K | Joback Method |
| vc | 0.894 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 594.57 | J/mol×K | 849.22 | Joback Method |
| cpg | 634.45 | J/mol×K | 1041.29 | Joback Method |
| cpg | 628.06 | J/mol×K | 1002.88 | Joback Method |
| cpg | 620.92 | J/mol×K | 964.46 | Joback Method |
| cpg | 612.99 | J/mol×K | 926.05 | Joback Method |
| cpg | 604.22 | J/mol×K | 887.63 | Joback Method |
| cpg | 640.13 | J/mol×K | 1079.70 | Joback Method |
| dvisc | 0.0000961 | Pa×s | 849.22 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001187 | Pa×s | 802.31 | Joback Method |
| dvisc | 0.0001505 | Pa×s | 755.41 | Joback Method |
| dvisc | 0.0001970 | Pa×s | 708.50 | Joback Method |
| dvisc | 0.0002678 | Pa×s | 661.60 | Joback Method |
| dvisc | 0.0003816 | Pa×s | 614.70 | Joback Method |
| dvisc | 0.0005764 | Pa×s | 567.79 | Joback Method |

# Sources

| | |
|---|---|
| **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=U370076&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |