# Diethylmalonic acid, 3,5-dichlorophenyl propyl ester

**Inchi:** InChI=1S/C16H20Cl2O4/c1-4-7-21-14(19)16(5-2,6-3)15(20)22-13-9-11(17)8-12(18)10-13

**InchiKey:** WKDHIXTZIUBCFD-UHFFFAOYSA-N

**Formula:** C16H20Cl2O4

**SMILES:** CCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1

**Mol. weight [g/mol]:** 347.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -311.87 | kJ/mol | Joback Method |
| hf | -689.81 | kJ/mol | Joback Method |
| hfus | 37.01 | kJ/mol | Joback Method |
| hvap | 80.60 | kJ/mol | Joback Method |
| log10ws | -5.12 | | Crippen Method |
| logp | 4.658 | | Crippen Method |
| mcvol | 251.900 | ml/mol | McGowan Method |
| pc | 1713.19 | kPa | Joback Method |
| rinpol | 2075.00 | | NIST Webbook |
| rinpol | 2075.00 | | NIST Webbook |
| tb | 826.33 | K | Joback Method |
| tc | 1044.31 | K | Joback Method |
| tf | 528.12 | K | Joback Method |
| vc | 0.959 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 700.42 | J/mol×K | 826.33 | Joback Method |
| cpg | 755.12 | J/mol×K | 1007.98 | Joback Method |
| cpg | 746.13 | J/mol×K | 971.65 | Joback Method |
| cpg | 736.19 | J/mol×K | 935.32 | Joback Method |
| cpg | 725.29 | J/mol×K | 898.99 | Joback Method |
| cpg | 713.37 | J/mol×K | 862.66 | Joback Method |
| cpg | 763.21 | J/mol×K | 1044.31 | Joback Method |
| dvisc | 0.0000580 | Pa×s | 826.33 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000735 | Pa×s | 776.63 | Joback Method |
| dvisc | 0.0000963 | Pa×s | 726.93 | Joback Method |
| dvisc | 0.0001313 | Pa×s | 677.22 | Joback Method |
| dvisc | 0.0001879 | Pa×s | 627.52 | Joback Method |
| dvisc | 0.0002861 | Pa×s | 577.82 | Joback Method |
| dvisc | 0.0004716 | Pa×s | 528.12 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370436&Units=SI |
| **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 |

# 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 |