# Diethylmalonic acid, isobutyl 2,4,5-trichlorophenyl ester

**Inchi:** InChI=1S/C17H21Cl3O4/c1-5-17(6-2,15(21)23-9-10(3)4)16(22)24-14-8-12(19)11(18)7-13

**InchiKey:** VTLRKRHFHFAQII-UHFFFAOYSA-N

**Formula:** C17H21Cl3O4

**SMILES:** CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1cc(Cl)c(Cl)cc1Cl

**Mol. weight [g/mol]:** 395.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -327.45 | kJ/mol | Joback Method |
| hf | -742.94 | kJ/mol | Joback Method |
| hfus | 39.89 | kJ/mol | Joback Method |
| hvap | 87.48 | kJ/mol | Joback Method |
| log10ws | -5.99 | | Crippen Method |
| logp | 5.558 | | Crippen Method |
| mcvol | 278.230 | ml/mol | McGowan Method |
| pc | 1530.66 | kPa | Joback Method |
| rinpol | 2317.00 | | NIST Webbook |
| rinpol | 2317.00 | | NIST Webbook |
| tb | 891.18 | K | Joback Method |
| tc | 1114.69 | K | Joback Method |
| tf | 566.83 | K | Joback Method |
| vc | 1.058 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 778.49 | J/mol×K | 891.18 | Joback Method |
| cpg | 790.52 | J/mol×K | 928.43 | Joback Method |
| cpg | 801.45 | J/mol×K | 965.68 | Joback Method |
| cpg | 811.32 | J/mol×K | 1002.93 | Joback Method |
| cpg | 820.17 | J/mol×K | 1040.19 | Joback Method |
| cpg | 828.03 | J/mol×K | 1077.44 | Joback Method |
| cpg | 834.93 | J/mol×K | 1114.69 | Joback Method |
| dvisc | 0.0003309 | Pa×s | 566.83 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001987 | Pa×s | 620.89 | Joback Method |
| dvisc | 0.0001295 | Pa×s | 674.95 | Joback Method |
| dvisc | 0.0000899 | Pa×s | 729.00 | Joback Method |
| dvisc | 0.0000657 | Pa×s | 783.06 | Joback Method |
| dvisc | 0.0000499 | Pa×s | 837.12 | Joback Method |
| dvisc | 0.0000393 | Pa×s | 891.18 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370530&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 |

# 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 |