# Dimethylmalonic acid, isohexyl pentachlorophenyl ester

**Inchi:** InChI=1S/C17H19Cl5O4/c1-8(2)6-5-7-25-15(23)17(3,4)16(24)26-14-12(21)10(19)9(18)11

**InchiKey:** IDEFHPCVLDDHPY-UHFFFAOYSA-N

**Formula:** C17H19Cl5O4

**SMILES:** CC(C)CCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl

**Mol. weight [g/mol]:** 464.60

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -370.57 | kJ/mol | Joback Method |
| hf | -797.36 | kJ/mol | Joback Method |
| hfus | 47.50 | kJ/mol | Joback Method |
| hvap | 97.58 | kJ/mol | Joback Method |
| log10ws | -7.36 | | Crippen Method |
| logp | 6.865 | | Crippen Method |
| mcvol | 302.710 | ml/mol | McGowan Method |
| pc | 1413.31 | kPa | Joback Method |
| rinpol | 2788.00 | | NIST Webbook |
| rinpol | 2788.00 | | NIST Webbook |
| tb | 976.00 | K | Joback Method |
| tc | 1209.23 | K | Joback Method |
| tf | 651.71 | K | Joback Method |
| vc | 1.155 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 815.09 | J/mol×K | 976.00 | Joback Method |
| cpg | 851.37 | J/mol×K | 1170.36 | Joback Method |
| cpg | 846.22 | J/mol×K | 1131.49 | Joback Method |
| cpg | 840.05 | J/mol×K | 1092.62 | Joback Method |
| cpg | 832.83 | J/mol×K | 1053.74 | Joback Method |
| cpg | 824.52 | J/mol×K | 1014.87 | Joback Method |
| cpg | 855.51 | J/mol×K | 1209.23 | Joback Method |
| dvisc | 0.0000286 | Pa×s | 976.00 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000354 | Pa×s | 921.95 | Joback Method |
| dvisc | 0.0000450 | Pa×s | 867.90 | Joback Method |
| dvisc | 0.0000591 | Pa×s | 813.86 | Joback Method |
| dvisc | 0.0000807 | Pa×s | 759.81 | Joback Method |
| dvisc | 0.0001155 | Pa×s | 705.76 | Joback Method |
| dvisc | 0.0001756 | Pa×s | 651.71 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U363928&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

| | |
|---|---|
| **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 |