# Diethylmalonic acid, dipentafluorobenzyl ester

**Inchi:** InChI=1S/C21H14F10O4/c1-3-21(4-2,19(32)34-5-7-9(22)13(26)17(30)14(27)10(7)23)20(
**InchiKey:** AXWJURRSJIOQFZ-UHFFFAOYSA-N
**Formula:** C21H14F10O4
**SMILES:** CCC(CC)(C(=O)OCc1c(F)c(F)c(F)c(F)c1F)C(=O)OCc1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 520.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2158.64 | kJ/mol | Joback Method |
| hf | -2577.86 | kJ/mol | Joback Method |
| hfus | 63.30 | kJ/mol | Joback Method |
| hvap | 82.36 | kJ/mol | Joback Method |
| log10ws | -8.61 | | Crippen Method |
| logp | 5.671 | | Crippen Method |
| mcvol | 291.810 | ml/mol | McGowan Method |
| pc | 1067.27 | kPa | Joback Method |
| rinpol | 2026.00 | | NIST Webbook |
| rinpol | 2026.00 | | NIST Webbook |
| tb | 925.09 | K | Joback Method |
| tc | 1133.14 | K | Joback Method |
| tf | 657.11 | K | Joback Method |
| vc | 1.212 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 900.68 | J/mol×K | 925.09 | Joback Method |
| cpg | 911.43 | J/mol×K | 959.76 | Joback Method |
| cpg | 921.05 | J/mol×K | 994.44 | Joback Method |
| cpg | 929.56 | J/mol×K | 1029.11 | Joback Method |
| cpg | 936.96 | J/mol×K | 1063.79 | Joback Method |
| cpg | 943.26 | J/mol×K | 1098.46 | Joback Method |
| cpg | 948.47 | J/mol×K | 1133.14 | 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=U370006&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |