# Diethylmalonic acid, 2-fluorophenyl nonyl ester

**Inchi:** InChI=1S/C22H33FO4/c1-4-7-8-9-10-11-14-17-26-20(24)22(5-2,6-3)21(25)27-19-16-13-1

**InchiKey:** NHYNGMMIUWUANQ-UHFFFAOYSA-N

**Formula:** C22H33FO4

**SMILES:** CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1F

**Mol. weight [g/mol]:** 380.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -422.67 | kJ/mol | Joback Method |
| hf | -966.81 | kJ/mol | Joback Method |
| hfus | 47.63 | kJ/mol | Joback Method |
| hvap | 83.70 | kJ/mol | Joback Method |
| log10ws | -6.60 | | Crippen Method |
| logp | 5.831 | | Crippen Method |
| mcvol | 313.730 | ml/mol | McGowan Method |
| pc | 1150.65 | kPa | Joback Method |
| rinpol | 2388.00 | | NIST Webbook |
| tb | 883.04 | K | Joback Method |
| tc | 1086.27 | K | Joback Method |
| tf | 523.97 | K | Joback Method |
| vc | 1.214 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1005.03 | J/mol×K | 883.04 | Joback Method |
| cpg | 1021.31 | J/mol×K | 916.91 | Joback Method |
| cpg | 1036.40 | J/mol×K | 950.78 | Joback Method |
| cpg | 1050.37 | J/mol×K | 984.65 | Joback Method |
| cpg | 1063.26 | J/mol×K | 1018.52 | Joback Method |
| cpg | 1075.10 | J/mol×K | 1052.40 | Joback Method |
| cpg | 1085.96 | J/mol×K | 1086.27 | Joback Method |

# Sources

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|---|---|
| **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=U370133&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |