# Diethylmalonic acid, 4-cyanophenyl octyl ester

**Inchi:** InChI=1S/C22H31NO4/c1-4-7-8-9-10-11-16-26-20(24)22(5-2,6-3)21(25)27-19-14-12-18(
**InchiKey:** DSAJTWSPDVTGTD-UHFFFAOYSA-N
**Formula:** C22H31NO4
**SMILES:** CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(C#N)cc1
**Mol. weight [g/mol]:** 373.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -94.68 | kJ/mol | Joback Method |
| hf | -605.82 | kJ/mol | Joback Method |
| hfus | 46.05 | kJ/mol | Joback Method |
| hvap | 95.00 | kJ/mol | Joback Method |
| log10ws | -6.20 | | Crippen Method |
| logp | 5.174 | | Crippen Method |
| mcvol | 313.340 | ml/mol | McGowan Method |
| pc | 1166.43 | kPa | Joback Method |
| rinpol | 2607.00 | | NIST Webbook |
| rinpol | 2607.00 | | NIST Webbook |
| tb | 985.85 | K | Joback Method |
| tc | 1209.67 | K | Joback Method |
| tf | 588.37 | K | Joback Method |
| vc | 1.222 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1020.51 | J/mol×K | 985.85 | Joback Method |
| cpg | 1033.93 | J/mol×K | 1023.15 | Joback Method |
| cpg | 1046.14 | J/mol×K | 1060.46 | Joback Method |
| cpg | 1057.19 | J/mol×K | 1097.76 | Joback Method |
| cpg | 1067.13 | J/mol×K | 1135.06 | Joback Method |
| cpg | 1076.04 | J/mol×K | 1172.37 | Joback Method |
| cpg | 1083.96 | J/mol×K | 1209.67 | 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=U369606&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 |
| **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 |