# Diethylmalonic acid, 4-cyanophenyl hexyl ester

**Inchi:** InChI=1S/C20H27NO4/c1-4-7-8-9-14-24-18(22)20(5-2,6-3)19(23)25-17-12-10-16(15-21)1

**InchiKey:** RMPZVJHGGWXLOV-UHFFFAOYSA-N

**Formula:** C20H27NO4

**SMILES:** CCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(C#N)cc1

**Mol. weight [g/mol]:** 345.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -111.52 | kJ/mol | Joback Method |
| hf | -564.54 | kJ/mol | Joback Method |
| hfus | 40.87 | kJ/mol | Joback Method |
| hvap | 90.55 | kJ/mol | Joback Method |
| log10ws | -5.36 | | Crippen Method |
| logp | 4.394 | | Crippen Method |
| mcvol | 285.160 | ml/mol | McGowan Method |
| pc | 1335.88 | kPa | Joback Method |
| rinpol | 2409.00 | | NIST Webbook |
| tb | 940.09 | K | Joback Method |
| tc | 1160.16 | K | Joback Method |
| tf | 565.83 | K | Joback Method |
| vc | 1.111 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 901.87 | J/mol×K | 940.09 | Joback Method |
| cpg | 914.91 | J/mol×K | 976.77 | Joback Method |
| cpg | 926.80 | J/mol×K | 1013.45 | Joback Method |
| cpg | 937.59 | J/mol×K | 1050.13 | Joback Method |
| cpg | 947.34 | J/mol×K | 1086.80 | Joback Method |
| cpg | 956.10 | J/mol×K | 1123.48 | Joback Method |
| cpg | 963.90 | J/mol×K | 1160.16 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U369604&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 |