# Isophthalic acid, 4-cyanophenyl hexyl ester

**Inchi:** InChI=1S/C21H21NO4/c1-2-3-4-5-13-25-20(23)17-7-6-8-18(14-17)21(24)26-19-11-9-16(
**InchiKey:** JTBHLZKQPIPDTK-UHFFFAOYSA-N
**Formula:** C21H21NO4
**SMILES:** CCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C#N)cc2)c1
**Mol. weight [g/mol]:** 351.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -3.16 | kJ/mol | Joback Method |
| hf | -351.37 | kJ/mol | Joback Method |
| hfus | 44.53 | kJ/mol | Joback Method |
| hvap | 97.01 | kJ/mol | Joback Method |
| log10ws | -6.25 | | Crippen Method |
| logp | 4.515 | | Crippen Method |
| mcvol | 275.490 | ml/mol | McGowan Method |
| pc | 1556.12 | kPa | Joback Method |
| rinpol | 3047.00 | | NIST Webbook |
| rinpol | 3047.00 | | NIST Webbook |
| tb | 997.86 | K | Joback Method |
| tc | 1234.42 | K | Joback Method |
| tf | 613.62 | K | Joback Method |
| vc | 1.069 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 850.53 | J/mol×K | 997.86 | Joback Method |
| cpg | 860.93 | J/mol×K | 1037.29 | Joback Method |
| cpg | 870.00 | J/mol×K | 1076.71 | Joback Method |
| cpg | 877.79 | J/mol×K | 1116.14 | Joback Method |
| cpg | 884.33 | J/mol×K | 1155.57 | Joback Method |
| cpg | 889.66 | J/mol×K | 1195.00 | Joback Method |
| cpg | 893.81 | J/mol×K | 1234.42 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U344492&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 |
| **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 |

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