# Pentafluoropropanoic acid, 4-cyanophenyl ester

**Inchi:** InChI=1S/C10H4F5NO2/c11-9(12,10(13,14)15)8(17)18-7-3-1-6(5-16)2-4-7/h1-4H
**InchiKey:** QAKWNVVBWJTGSV-UHFFFAOYSA-N
**Formula:** C10H4F5NO2
**SMILES:** N#Cc1ccc(OC(=O)C(F)(F)C(F)(F)F)cc1
**Mol. weight [g/mol]:** 265.14

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -933.01 | kJ/mol | Joback Method |
| hf | -1102.64 | kJ/mol | Joback Method |
| hfus | 20.17 | kJ/mol | Joback Method |
| hvap | 53.75 | kJ/mol | Joback Method |
| log10ws | -3.53 | | Crippen Method |
| logp | 2.661 | | Crippen Method |
| mcvol | 145.670 | ml/mol | McGowan Method |
| pc | 2431.44 | kPa | Joback Method |
| rinpol | 938.00 | | NIST Webbook |
| tb | 628.12 | K | Joback Method |
| tc | 831.50 | K | Joback Method |
| tf | 386.34 | K | Joback Method |
| vc | 0.606 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 371.03 | J/mol×K | 628.12 | Joback Method |
| cpg | 380.02 | J/mol×K | 662.02 | Joback Method |
| cpg | 388.25 | J/mol×K | 695.91 | Joback Method |
| cpg | 395.76 | J/mol×K | 729.81 | Joback Method |
| cpg | 402.61 | J/mol×K | 763.71 | Joback Method |
| cpg | 408.85 | J/mol×K | 797.61 | Joback Method |
| cpg | 414.51 | J/mol×K | 831.50 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U308004&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 |