# 2,2,3,3-Tetrafluoropropionitrile

**Inchi:** InChI=1S/C3HF4N/c4-2(5)3(6,7)1-8/h2H
**InchiKey:** PIORIRQBACOORT-UHFFFAOYSA-N
**Formula:** C3HF4N
**SMILES:** N#CC(F)(F)C(F)F
**Mol. weight [g/mol]:** 127.04
**CAS:** 431-32-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -671.28 | kJ/mol | Joback Method |
| hf | -738.84 | kJ/mol | Joback Method |
| hfus | 6.42 | kJ/mol | Joback Method |
| hvap | 27.80 | kJ/mol | Joback Method |
| log10ws | -1.57 | | Crippen Method |
| logp | 1.410 | | Crippen Method |
| mcvol | 61.590 | ml/mol | McGowan Method |
| pc | 3526.27 | kPa | Joback Method |
| tb | 314.00 ± 1.00 | K | NIST Webbook |
| tc | 532.03 | K | Joback Method |
| tf | 178.34 | K | Joback Method |
| vc | 0.284 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 120.95 | J/mol×K | 363.53 | Joback Method |
| cpg | 126.20 | J/mol×K | 391.61 | Joback Method |
| cpg | 131.10 | J/mol×K | 419.70 | Joback Method |
| cpg | 135.68 | J/mol×K | 447.78 | Joback Method |
| cpg | 139.94 | J/mol×K | 475.86 | Joback Method |
| cpg | 143.91 | J/mol×K | 503.95 | Joback Method |
| cpg | 147.59 | J/mol×K | 532.03 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C431323&Units=SI |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |