# 2,3,4,6-Tetrafluoronitrobenzene

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|---|---|
| **Other names:** | Benzene, 1,2,3,5-tetrafluoro-4-nitro- |
| | 1,2,3,5-tetrafluoro-4-nitrobenzene |
| **Inchi:** | InChI=1S/C6HF4NO2/c7-2-1-3(8)6(11(12)13)5(10)4(2)9/h1H |
| **InchiKey:** | FDLCUAUNAWWSBX-UHFFFAOYSA-N |
| **Formula:** | C6HF4NO2 |
| **SMILES:** | O=[N+]([O-])c1c(F)cc(F)c(F)c1F |
| **Mol. weight [g/mol]:** | 195.07 |
| **CAS:** | 314-41-0 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -670.16 | kJ/mol | Joback Method |
| hf | -771.72 | kJ/mol | Joback Method |
| hfus | 27.46 | kJ/mol | Joback Method |
| hvap | 47.20 | kJ/mol | Joback Method |
| log10ws | -3.45 | | Crippen Method |
| logp | 2.151 | | Crippen Method |
| mcvol | 96.140 | ml/mol | McGowan Method |
| pc | 3497.14 | kPa | Joback Method |
| tb | 532.20 | K | Joback Method |
| tc | 741.46 | K | Joback Method |
| tf | 379.85 | K | Joback Method |
| vc | 0.417 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 210.19 | J/mol×K | 532.20 | Joback Method |
| cpg | 217.12 | J/mol×K | 567.08 | Joback Method |
| cpg | 223.65 | J/mol×K | 601.95 | Joback Method |
| cpg | 229.80 | J/mol×K | 636.83 | Joback Method |
| cpg | 235.58 | J/mol×K | 671.71 | Joback Method |
| cpg | 240.98 | J/mol×K | 706.59 | Joback Method |
| cpg | 246.01 | J/mol×K | 741.46 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 351.50 ± 0.50 | K | 2.70 | NIST Webbook |

# 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=C314410&Units=SI |

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