# Carbonic acid, propyl 2-nitro-5-fluorophenyl ester

**Inchi:** InChI=1S/C10H10FNO5/c1-2-5-16-10(13)17-9-6-7(11)3-4-8(9)12(14)15/h3-4,6H,2,5H2,1

**InchiKey:** SJPJWMQEQDHZIG-UHFFFAOYSA-N

**Formula:** C10H10FNO5

**SMILES:** CCCOC(=O)Oc1cc(F)ccc1[N+](=O)[O-]

**Mol. weight [g/mol]:** 243.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -371.71 | kJ/mol | Joback Method |
| hf | -620.03 | kJ/mol | Joback Method |
| hfus | 33.33 | kJ/mol | Joback Method |
| hvap | 68.79 | kJ/mol | Joback Method |
| log10ws | -3.67 | | Crippen Method |
| logp | 2.659 | | Crippen Method |
| mcvol | 160.500 | ml/mol | McGowan Method |
| pc | 2826.33 | kPa | Joback Method |
| rinpol | 1613.00 | | NIST Webbook |
| tb | 714.66 | K | Joback Method |
| tc | 939.38 | K | Joback Method |
| tf | 492.51 | K | Joback Method |
| vc | 0.629 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 425.58 | J/mol×K | 714.66 | Joback Method |
| cpg | 436.77 | J/mol×K | 752.11 | Joback Method |
| cpg | 447.14 | J/mol×K | 789.57 | Joback Method |
| cpg | 456.68 | J/mol×K | 827.02 | Joback Method |
| cpg | 465.40 | J/mol×K | 864.47 | Joback Method |
| cpg | 473.28 | J/mol×K | 901.93 | Joback Method |
| cpg | 480.32 | J/mol×K | 939.38 | Joback Method |

# Sources

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|---|---|
| **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=U357820&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |