# Propanoic acid, 2,2-dimethyl-, 4-nitrophenyl ester

**Other names:** 2,2-Dimethylpropanoic acid, 4-nitrophenyl ester
p-nitrophenyl pivalate

**Inchi:** InChI=1S/C11H13NO4/c1-11(2,3)10(13)16-9-6-4-8(5-7-9)12(14)15/h4-7H,1-3H3

**InchiKey:** QADVJDGFQGNSIF-UHFFFAOYSA-N

**Formula:** C11H13NO4

**SMILES:** CC(C)(C)C(=O)Oc1ccc([N+](=O)[O-])cc1

**Mol. weight [g/mol]:** 223.23

**CAS:** 4195-17-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -51.01 | kJ/mol | Joback Method |
| hf | -309.62 | kJ/mol | Joback Method |
| hfus | 24.63 | kJ/mol | Joback Method |
| hvap | 67.47 | kJ/mol | Joback Method |
| log10ws | -3.45 | | Crippen Method |
| logp | 2.546 | | Crippen Method |
| mcvol | 166.950 | ml/mol | McGowan Method |
| pc | 2826.33 | kPa | Joback Method |
| rinpol | 1602.00 | | NIST Webbook |
| tb | 707.64 | K | Joback Method |
| tc | 953.76 | K | Joback Method |
| tf | 470.86 | K | Joback Method |
| vc | 0.638 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 448.61 | J/mol×K | 707.64 | Joback Method |
| cpg | 461.74 | J/mol×K | 748.66 | Joback Method |
| cpg | 473.77 | J/mol×K | 789.68 | Joback Method |
| cpg | 484.76 | J/mol×K | 830.70 | Joback Method |
| cpg | 494.78 | J/mol×K | 871.72 | Joback Method |
| cpg | 503.88 | J/mol×K | 912.74 | Joback Method |

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|---|---|---|---|---|
| cpg | 512.13 | J/mol×K | 953.76 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4195179&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |