# Phenylacetic acid, 4-nitrophenyl ester

**Inchi:** InChI=1S/C14H11NO4/c16-14(10-11-4-2-1-3-5-11)19-13-8-6-12(7-9-13)15(17)18/h1-9H,
**InchiKey:** SSYHGZXPSAYXLS-UHFFFAOYSA-N
**Formula:** C14H11NO4
**SMILES:** O=C(Cc1ccccc1)Oc1ccc([N+](=O)[O-])cc1
**Mol. weight [g/mol]:** 257.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 83.82 | kJ/mol | Joback Method |
| hf | -126.26 | kJ/mol | Joback Method |
| hfus | 33.86 | kJ/mol | Joback Method |
| hvap | 77.72 | kJ/mol | Joback Method |
| log10ws | -4.05 | | Crippen Method |
| logp | 2.743 | | Crippen Method |
| mcvol | 185.460 | ml/mol | McGowan Method |
| pc | 2899.85 | kPa | Joback Method |
| rinpol | 2118.00 | | NIST Webbook |
| rinpol | 2118.00 | | NIST Webbook |
| tb | 806.19 | K | Joback Method |
| tc | 1067.65 | K | Joback Method |
| tf | 528.67 | K | Joback Method |
| vc | 0.710 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 510.55 | J/mol×K | 806.19 | Joback Method |
| cpg | 522.67 | J/mol×K | 849.77 | Joback Method |
| cpg | 533.54 | J/mol×K | 893.34 | Joback Method |
| cpg | 543.22 | J/mol×K | 936.92 | Joback Method |
| cpg | 551.78 | J/mol×K | 980.50 | Joback Method |
| cpg | 559.28 | J/mol×K | 1024.08 | Joback Method |
| cpg | 565.80 | J/mol×K | 1067.65 | 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=U307536&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |