# 4-Nitrobenzoic acid, oct-3-en-2-yl ester

**Inchi:** InChI=1S/C15H19NO4/c1-3-4-5-6-7-12(2)20-15(17)13-8-10-14(11-9-13)16(18)19/h6-12H
**InchiKey:** LXVKUUDHSWMVOA-VOTSOKGWSA-N
**Formula:** C15H19NO4
**SMILES:** CCCCC=CC(C)OC(=O)c1ccc([N+](=O)[O-])cc1
**Mol. weight [g/mol]:** 277.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 57.61 | kJ/mol | Joback Method |
| hf | -271.49 | kJ/mol | Joback Method |
| hfus | 39.09 | kJ/mol | Joback Method |
| hvap | 77.24 | kJ/mol | Joback Method |
| log10ws | -5.26 | | Crippen Method |
| logp | 3.886 | | Crippen Method |
| mcvol | 219.010 | ml/mol | McGowan Method |
| pc | 2021.76 | kPa | Joback Method |
| rinpol | 2023.00 | | NIST Webbook |
| tb | 806.11 | K | Joback Method |
| tc | 1035.35 | K | Joback Method |
| tf | 493.44 | K | Joback Method |
| vc | 0.848 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 634.58 | J/mol×K | 806.11 | Joback Method |
| cpg | 648.57 | J/mol×K | 844.32 | Joback Method |
| cpg | 661.51 | J/mol×K | 882.52 | Joback Method |
| cpg | 673.46 | J/mol×K | 920.73 | Joback Method |
| cpg | 684.47 | J/mol×K | 958.94 | Joback Method |
| cpg | 694.61 | J/mol×K | 997.14 | Joback Method |
| cpg | 703.92 | J/mol×K | 1035.35 | 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=U299268&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 |