# Benzeneacetic acid, 4-nitro-, 2-methyloct-5-yn-4-yl ester

**Inchi:** InChI=1S/C17H21NO4/c1-4-5-6-16(11-13(2)3)22-17(19)12-14-7-9-15(10-8-14)18(20)21/
**InchiKey:** ASAYLLCDIXXUSW-UHFFFAOYSA-N
**Formula:** C17H21NO4
**SMILES:** CCC#CC(CC(C)C)OC(=O)Cc1ccc([N+](=O)[O-])cc1
**Mol. weight [g/mol]:** 303.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 194.59 | kJ/mol | Joback Method |
| hf | -162.97 | kJ/mol | Joback Method |
| hfus | 43.66 | kJ/mol | Joback Method |
| hvap | 83.50 | kJ/mol | Joback Method |
| log10ws | -5.22 | | Crippen Method |
| logp | 3.509 | | Crippen Method |
| mcvol | 242.890 | ml/mol | McGowan Method |
| pc | 1890.36 | kPa | Joback Method |
| rinpol | 2236.00 | | NIST Webbook |
| rinpol | 2236.00 | | NIST Webbook |
| tb | 856.27 | K | Joback Method |
| tc | 1095.10 | K | Joback Method |
| tf | 612.16 | K | Joback Method |
| vc | 0.935 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 721.89 | J/mol×K | 856.27 | Joback Method |
| cpg | 736.38 | J/mol×K | 896.07 | Joback Method |
| cpg | 749.64 | J/mol×K | 935.88 | Joback Method |
| cpg | 761.71 | J/mol×K | 975.68 | Joback Method |
| cpg | 772.63 | J/mol×K | 1015.49 | Joback Method |
| cpg | 782.46 | J/mol×K | 1055.29 | Joback Method |
| cpg | 791.24 | J/mol×K | 1095.10 | 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=U406979&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 |

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