# Butanoic acid, pent-2-en-4-ynyl ester

**Inchi:** InChI=1S/C9H12O2/c1-3-5-6-8-11-9(10)7-4-2/h1,5-6H,4,7-8H2,2H3
**InchiKey:** UTBJMMZGNZOAAW-UHFFFAOYSA-N
**Formula:** C9H12O2
**SMILES:** C#CC=CCOC(=O)CCC
**Mol. weight [g/mol]:** 152.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 94.27 | kJ/mol | Joback Method |
| hf | -64.77 | kJ/mol | Joback Method |
| hfus | 25.03 | kJ/mol | Joback Method |
| hvap | 44.60 | kJ/mol | Joback Method |
| log10ws | -2.10 | | Crippen Method |
| logp | 1.519 | | Crippen Method |
| mcvol | 132.210 | ml/mol | McGowan Method |
| pc | 2966.57 | kPa | Joback Method |
| tb | 475.89 | K | Joback Method |
| tc | 670.01 | K | Joback Method |
| tf | 305.24 | K | Joback Method |
| vc | 0.505 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 273.67 | J/mol×K | 475.89 | Joback Method |
| cpg | 285.17 | J/mol×K | 508.24 | Joback Method |
| cpg | 296.12 | J/mol×K | 540.60 | Joback Method |
| cpg | 306.53 | J/mol×K | 572.95 | Joback Method |
| cpg | 316.42 | J/mol×K | 605.31 | Joback Method |
| cpg | 325.81 | J/mol×K | 637.66 | Joback Method |
| cpg | 334.72 | J/mol×K | 670.01 | Joback Method |

# Sources

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|---|---|
| **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=U299119&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |