# 2-PROPYNOIC ACID, 3-PHENYL-, ETHYL ESTER

**Other names:** 2-Propynoic acid, 3-phenyl-, ethyl ester
3-Phenyl-2-propynoic acid ethyl ester
Ethyl 3-phenylpropiolate
Ethyl 3-phenylpropynoate
Ethyl phenylacetylenecarboxylate
Ethyl phenylpropriolate
Ethyl phenylpropynoate
NSC 41566
Phenylacetylene monocarboxylic acid ethyl ester
Propiolic acid, phenyl-, ethyl ester
ethyl 3-phenylprop-2-ynoate

**Inchi:** InChI=1S/C11H10O2/c1-2-13-11(12)9-8-10-6-4-3-5-7-10/h3-7H,2H2,1H3

**InchiKey:** ACJOYTKWHPEIHW-UHFFFAOYSA-N

**Formula:** C11H10O2

**SMILES:** CCOC(=O)C#Cc1ccccc1

**Mol. weight [g/mol]:** 174.20

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.4137 | | Cheméo Relay (1.0) |
| chl | -5606.10 | kJ/mol | NIST Webbook |
| hf | -87.60 | kJ/mol | Cheméo Relay (1.0) |
| hfl | -151.70 ± 5.00 | kJ/mol | NIST Webbook |
| hfl | 189.00 | kJ/mol | NIST Webbook |
| hfus | 24.20 | kJ/mol | Joback Method |
| hvap | 69.41 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.78 | eV | Cheméo Relay (1.0) |
| log10ws | -2.68 | | Cheméo Relay (1.0) |
| logp | 1.601 | | Crippen Method |
| mcvol | 140.930 | ml/mol | McGowan Method |
| pc | 3314.37 | kPa | Joback Method |
| tb | 538.00 ± 5.00 | K | NIST Webbook |
| tb | 538.20 | K | NIST Webbook |
| tc | 713.47 | K | Cheméo Relay (1.0) |
| tf | 285.66 | K | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 308.87 | J/mol×K | 563.05 | Joback Method |
| cpg | 322.37 | J/mol×K | 602.45 | Joback Method |
| cpg | 335.03 | J/mol×K | 641.84 | Joback Method |
| cpg | 346.86 | J/mol×K | 681.24 | Joback Method |
| cpg | 357.87 | J/mol×K | 720.64 | Joback Method |
| cpg | 368.10 | J/mol×K | 760.03 | Joback Method |
| cpg | 377.57 | J/mol×K | 799.43 | Joback Method |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C2216946&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

**af:** Acentric Factor
**chl:** Standard liquid enthalpy of combustion
**cpg:** Ideal gas heat capacity
**hf:** Enthalpy of formation at standard conditions
**hfl:** Liquid phase enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**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