# 2-NONENOIC ACID, ETHYL ESTER

**Other names:** Ethyl 2-nonenoate
ethyl non-2-enoate
**Inchi:** InChI=1S/C11H20O2/c1-3-5-6-7-8-9-10-11(12)13-4-2/h9-10H,3-8H2,1-2H3/b10-9+
**InchiKey:** ZCSDUGXKKBIICL-MDZDMXLPSA-N
**Formula:** C11H20O2
**SMILES:** CCCCCC/C=C/C(=O)OCC
**Mol. weight [g/mol]:** 184.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5880 | | Cheméo Relay (1.0) |
| gf | -111.96 | kJ/mol | Joback Method |
| hf | -482.43 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 27.24 | kJ/mol | Joback Method |
| hvap | 63.67 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.55 | eV | Cheméo Relay (1.0) |
| log10ws | -4.28 | | Cheméo Relay (1.0) |
| logp | 3.076 | | Crippen Method |
| mcvol | 168.990 | ml/mol | McGowan Method |
| pc | 2111.94 | kPa | Joback Method |
| tb | 487.27 | K | Cheméo Relay (1.0) |
| tc | 675.64 | K | Cheméo Relay (1.0) |
| tf | 226.57 | K | Cheméo Relay (1.0) |
| vc | 0.628 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 397.35 | J/mol×K | 531.53 | Joback Method |
| cpg | 411.96 | J/mol×K | 561.21 | Joback Method |
| cpg | 425.95 | J/mol×K | 590.89 | Joback Method |
| cpg | 439.33 | J/mol×K | 620.57 | Joback Method |
| cpg | 452.12 | J/mol×K | 650.25 | Joback Method |
| cpg | 464.33 | J/mol×K | 679.93 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 475.98 | J/mol×K | 709.61 | Joback Method |
| dvisc | 0.0029775 | Pa×s | 280.81 | Joback Method |
| dvisc | 0.0013650 | Pa×s | 322.60 | Joback Method |
| dvisc | 0.0007484 | Pa×s | 364.38 | Joback Method |
| dvisc | 0.0004643 | Pa×s | 406.17 | Joback Method |
| dvisc | 0.0003149 | Pa×s | 447.96 | Joback Method |
| dvisc | 0.0002282 | Pa×s | 489.74 | Joback Method |
| dvisc | 0.0001740 | Pa×s | 531.53 | Joback Method |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C17463013&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

# Legend

**af:** Acentric Factor
**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**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
**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
**vc:** Critical Volume