# Allyl acetate

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|---|---|
| **Other names:** | 2-Propenyl acetate |
| | 2-Propenyl ester of acetic acid |
| | 2-Propenyl ethanoate |
| | 3-Acetoxy-1-propene |
| | 3-Acetoxypropene |
| | Acetic acid, 2-propen-1-yl ester |
| | Acetic acid, 2-propenyl ester |
| | Acetic acid, allyl ester |
| | CH2=C(CH3)OC(=O)CH3 |
| | NSC 7612 |
| | UN 2333 |
| **Inchi:** | InChI=1S/C5H8O2/c1-3-4-7-5(2)6/h3H,1,4H2,2H3 |
| **InchiKey:** | FWZUNOYOVVKUNF-UHFFFAOYSA-N |
| **Formula:** | C5H8O2 |
| **SMILES:** | C=CCOC(C)=O |
| **Mol. weight [g/mol]:** | 100.12 |
| **CAS:** | 591-87-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -154.86 | kJ/mol | Joback Method |
| hf | -265.90 | kJ/mol | Joback Method |
| hfus | 10.21 | kJ/mol | Joback Method |
| hvap | 35.21 | kJ/mol | Joback Method |
| ie | 9.74 ± 0.05 | eV | NIST Webbook |
| ie | 9.81 | eV | NIST Webbook |
| ie | 9.80 | eV | NIST Webbook |
| log10ws | -0.63 | | Crippen Method |
| logp | 0.735 | | Crippen Method |
| mcvol | 84.450 | ml/mol | McGowan Method |
| pc | 3857.88 | kPa | Joback Method |
| rinpol | 681.00 | | NIST Webbook |
| rinpol | 656.00 | | NIST Webbook |
| rinpol | 670.00 | | NIST Webbook |
| rinpol | 670.00 | | NIST Webbook |
| rinpol | 658.00 | | NIST Webbook |
| rinpol | 680.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 675.00 | | NIST Webbook |
| rinpol | 670.00 | | NIST Webbook |
| rinpol | 675.00 | | NIST Webbook |
| ripol | 1023.00 | | NIST Webbook |
| ripol | 1010.00 | | NIST Webbook |
| ripol | 1010.00 | | NIST Webbook |
| ripol | 1025.00 | | NIST Webbook |
| ripol | 1010.00 | | NIST Webbook |
| ripol | 1023.00 | | NIST Webbook |
| ripol | 1014.00 | | NIST Webbook |
| tb | 377.70 ± 1.00 | K | NIST Webbook |
| tb | 378.00 | K | NIST Webbook |
| tb | 376.70 | K | NIST Webbook |
| tc | 569.17 | K | Joback Method |
| tf | 216.51 | K | Joback Method |
| vc | 0.321 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 149.35 | J/mol×K | 386.77 | Joback Method |
| cpg | 157.10 | J/mol×K | 417.17 | Joback Method |
| cpg | 164.59 | J/mol×K | 447.57 | Joback Method |
| cpg | 171.82 | J/mol×K | 477.97 | Joback Method |
| cpg | 178.80 | J/mol×K | 508.37 | Joback Method |
| cpg | 185.52 | J/mol×K | 538.77 | Joback Method |
| cpg | 191.98 | J/mol×K | 569.17 | Joback Method |
| cpl | 184.10 | J/mol×K | 298.00 | NIST Webbook |
| dvisc | 0.0024241 | Pa×s | 216.51 | Joback Method |
| dvisc | 0.0013568 | Pa×s | 244.89 | Joback Method |
| dvisc | 0.0008567 | Pa×s | 273.26 | Joback Method |
| dvisc | 0.0005898 | Pa×s | 301.64 | Joback Method |
| dvisc | 0.0004330 | Pa×s | 330.02 | Joback Method |
| dvisc | 0.0003338 | Pa×s | 358.39 | Joback Method |
| dvisc | 0.0002673 | Pa×s | 386.77 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 6.11072e+01 |
| Coeff. B | -6.21372e+03 |
| Coeff. C | -6.89444e+00 |
| Coeff. D | 5.98005e-06 |
| Temperature range (K), min. | 138.00 |
| Temperature range (K), max. | 559.00 |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C591877&Units=SI |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1168 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol1168.mol |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase 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 |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |

| | |
|---|---|
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |