

1-Undecanol, acetate

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| Other names: | Acetic acid undecyl ester Undecyl acetate Undecyl alcohol, acetate acetic acid, undecyl ester n-Undecyl acetate undecanyl acetate undecyl ethanoate |
| Inchi: | InChI=1S/C13H26O2/c1-3-4-5-6-7-8-9-10-11-12-15-13(2)14/h3-12H2,1-2H3 |
| InchiKey: | CKQGCFDQIFZFA-UHFFFAOYSA-N |
| Formula: | C13H26O2 |
| SMILES: | CCCCCCCCCCCOC(C)=O |
| Mol. weight [g/mol]: | 214.34 |
| CAS: | 1731-81-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -175.34 | kJ/mol | Joback Method |
| hf | -556.45 | kJ/mol | Joback Method |
| hfus | 32.21 | kJ/mol | Joback Method |
| hvap | 53.69 | kJ/mol | Joback Method |
| log10ws | -4.13 | | Crippen Method |
| logp | 4.080 | | Crippen Method |
| mcvol | 201.470 | ml/mol | McGowan Method |
| pc | 1707.53 | kPa | Joback Method |
| rinpol | 1487.00 | | NIST Webbook |
| rinpol | 1507.60 | | NIST Webbook |
| rinpol | 1519.00 | | NIST Webbook |
| rinpol | 1498.00 | | NIST Webbook |
| rinpol | 1483.00 | | NIST Webbook |
| rinpol | 1493.00 | | NIST Webbook |
| ripol | 1775.00 | | NIST Webbook |
| ripol | 1802.00 | | NIST Webbook |
| tb | 573.13 | K | Joback Method |
| tc | 741.92 | K | Joback Method |
| tf | 308.43 | K | Joback Method |
| vc | 0.787 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|--|
| cpg | 514.80 | J/molxK | 573.13 | Joback Method |
| cpg | 546.77 | J/molxK | 629.39 | Joback Method |
| cpg | 561.79 | J/molxK | 657.52 | Joback Method |
| cpg | 576.19 | J/molxK | 685.66 | Joback Method |
| cpg | 589.97 | J/molxK | 713.79 | Joback Method |
| cpg | 603.14 | J/molxK | 741.92 | Joback Method |
| cpg | 531.11 | J/molxK | 601.26 | Joback Method |
| dvisc | 0.0013589 | Paxs | 352.55 | Joback Method |
| dvisc | 0.0007456 | Paxs | 396.66 | Joback Method |
| dvisc | 0.0004613 | Paxs | 440.78 | Joback Method |
| dvisc | 0.0003115 | Paxs | 484.90 | Joback Method |
| dvisc | 0.0002245 | Paxs | 529.01 | Joback Method |
| dvisc | 0.0029408 | Paxs | 308.43 | Joback Method |
| dvisc | 0.0001702 | Paxs | 573.13 | Joback Method |
| pvap | 0.01 | kPa | 329.40 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
| pvap | 8.29e-03 | kPa | 326.30 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
| pvap | 6.32e-03 | kPa | 323.30 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
| pvap | 4.99e-03 | kPa | 320.30 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |

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| pvap | 3.76e-03 | kPa | 317.30 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
| pvap | 2.98e-03 | kPa | 314.30 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
| pvap | 2.26e-03 | kPa | 311.20 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
| pvap | 1.67e-03 | kPa | 308.20 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
| pvap | 1.23e-03 | kPa | 305.20 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
| pvap | 9.50e-04 | kPa | 302.10 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
| pvap | 7.10e-04 | kPa | 299.00 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
| pvap | 4.90e-04 | kPa | 296.00 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
| pvap | 3.70e-04 | kPa | 292.90 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |

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|------|----------|-----|--------|--|
| pvap | 2.40e-04 | kPa | 288.90 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates |
|------|----------|-----|--------|--|

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.76319e+01 |
| Coeff. B | -5.64569e+03 |
| Coeff. C | -9.38140e+01 |
| Temperature range (K), min. | 419.32 |
| Temperature range (K), max. | 552.05 |

Sources

Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl acetates:

Joback Method:

KDB:

McGowan Method:

NIST Webbook:

The Yaws Handbook of Vapor Pressure:

Crippen Method:

Crippen Method:

<https://www.doi.org/10.1016/j.jct.2005.08.003>

https://en.wikipedia.org/wiki/Joback_method

<https://www.thermo.com/files/research/kdb/mol/mol1133.mol>

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1731813&Units=SI>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

| | |
|---------------|--|
| 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 |

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|-----------------|---|
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccvol: | 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 |

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