# (E)-3-Tridecen-2-yl acetate

**Inchi:** InChI=1S/C15H28O2/c1-4-5-6-7-8-9-10-11-12-13-14(2)17-15(3)16/h12-14H,4-11H2,1-3H
**InchiKey:** RGNGININXSUPKY-OUKQBFOZSA-N
**Formula:** C15H28O2
**SMILES:** CCCCCCCCCC=CC(C)OC(C)=O
**Mol. weight [g/mol]:** 240.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -80.72 | kJ/mol | Joback Method |
| hf | -485.79 | kJ/mol | Joback Method |
| hfus | 34.07 | kJ/mol | Joback Method |
| hvap | 57.71 | kJ/mol | Joback Method |
| log10ws | -4.93 | | Crippen Method |
| logp | 4.635 | | Crippen Method |
| mcvol | 225.350 | ml/mol | McGowan Method |
| pc | 1535.46 | kPa | Joback Method |
| rinpol | 1620.00 | | NIST Webbook |
| ripol | 1900.00 | | NIST Webbook |
| tb | 622.61 | K | Joback Method |
| tc | 798.28 | K | Joback Method |
| tf | 310.89 | K | Joback Method |
| vc | 0.874 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 600.96 | J/mol×K | 622.61 | Joback Method |
| cpg | 618.28 | J/mol×K | 651.89 | Joback Method |
| cpg | 634.82 | J/mol×K | 681.17 | Joback Method |
| cpg | 650.60 | J/mol×K | 710.44 | Joback Method |
| cpg | 665.65 | J/mol×K | 739.72 | Joback Method |
| cpg | 679.98 | J/mol×K | 769.00 | Joback Method |
| cpg | 693.62 | J/mol×K | 798.28 | Joback Method |
| dvisc | 0.0032461 | Pa×s | 310.89 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0012311 | Pa×s | 362.84 | Joback Method |
| dvisc | 0.0005952 | Pa×s | 414.80 | Joback Method |
| dvisc | 0.0003383 | Pa×s | 466.75 | Joback Method |
| dvisc | 0.0002154 | Pa×s | 518.70 | Joback Method |
| dvisc | 0.0001488 | Pa×s | 570.66 | Joback Method |
| dvisc | 0.0001094 | Pa×s | 622.61 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R203473&Units=SI |

# 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 |
| **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 |
| **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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