# E-3-TETRADECEN-1-OL ACETATE

**Other names:** E-3-tetradecenyl acetate
**Inchi:** InChI=1S/C16H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-16(2)17/h12-13H,3-11,14-1
**InchiKey:** YUOMITSDDKQODR-OUKQBFOZSA-N
**Formula:** C16H30O2
**SMILES:** CCCCCCCCCC/C=C/CCOC(C)=O
**Mol. weight [g/mol]:** 254.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.7334 | | Cheméo Relay (1.0) |
| gf | -69.86 | kJ/mol | Joback Method |
| hf | -599.97 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 40.18 | kJ/mol | Joback Method |
| hvap | 87.34 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.98 | eV | Cheméo Relay (1.0) |
| log10ws | -5.39 | | Cheméo Relay (1.0) |
| logp | 5.027 | | Crippen Method |
| mcvol | 239.440 | ml/mol | McGowan Method |
| pc | 1417.57 | kPa | Joback Method |
| rinpol | 1796.00 | | NIST Webbook |
| rinpol | 1796.00 | | NIST Webbook |
| ripol | 2104.00 | | NIST Webbook |
| ripol | 2104.00 | | NIST Webbook |
| tb | 559.78 | K | Cheméo Relay (1.0) |
| tc | 735.47 | K | Cheméo Relay (1.0) |
| tf | 262.26 | K | Cheméo Relay (1.0) |
| vc | 0.899 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 655.12 | J/mol×K | 645.93 | Joback Method |
| cpg | 748.76 | J/mol×K | 818.34 | Joback Method |
| cpg | 734.94 | J/mol×K | 789.61 | Joback Method |

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|---|---|---|---|---|
| cpg | 720.44 | J/mol×K | 760.87 | Joback Method |
| cpg | 705.23 | J/mol×K | 732.14 | Joback Method |
| cpg | 689.29 | J/mol×K | 703.40 | Joback Method |
| cpg | 672.59 | J/mol×K | 674.67 | Joback Method |
| dvisc | 0.0002997 | Pa×s | 491.54 | Joback Method |
| dvisc | 0.0001048 | Pa×s | 645.93 | Joback Method |
| dvisc | 0.0001400 | Pa×s | 594.47 | Joback Method |
| dvisc | 0.0001976 | Pa×s | 543.01 | Joback Method |
| dvisc | 0.0022449 | Pa×s | 337.16 | Joback Method |
| dvisc | 0.0005012 | Pa×s | 440.08 | Joback Method |
| dvisc | 0.0009605 | Pa×s | 388.62 | Joback Method |

# Sources

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|---|---|
| **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 |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U130811&Units=SI |

# 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 |
| **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 |