# E-11,13-DIMETHYL-12-TETRADECEN-1-OL ACETATE

**Inchi:** InChI=1S/C18H34O2/c1-16(2)15-17(3)13-11-9-7-5-6-8-10-12-14-20-18(4)19/h15,17H,5-1

**InchiKey:** MNUWBCKALSZWEW-UHFFFAOYSA-N

**Formula:** C18H34O2

**SMILES:** CC(=O)OCCCCCCCCCCCC(C)C=C(C)C

**Mol. weight [g/mol]:** 282.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.7827 | | Cheméo Relay (1.0) |
| hf | -664.35 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 40.53 | kJ/mol | Joback Method |
| hvap | 89.28 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.51 | eV | Cheméo Relay (1.0) |
| log10ws | -5.77 | | Cheméo Relay (1.0) |
| logp | 5.663 | | Crippen Method |
| mcvol | 267.620 | ml/mol | McGowan Method |
| pc | 1244.21 | kPa | Joback Method |
| rinpol | 1955.10 | | NIST Webbook |
| rinpol | 1955.10 | | NIST Webbook |
| tb | 576.22 | K | Cheméo Relay (1.0) |
| tc | 746.28 | K | Cheméo Relay (1.0) |
| tf | 277.66 | K | Cheméo Relay (1.0) |
| vc | 1.000 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 768.10 | J/mol×K | 691.13 | Joback Method |
| cpg | 786.83 | J/mol×K | 720.50 | Joback Method |
| cpg | 804.68 | J/mol×K | 749.87 | Joback Method |
| cpg | 821.68 | J/mol×K | 779.23 | Joback Method |
| cpg | 837.85 | J/mol×K | 808.60 | Joback Method |
| cpg | 853.24 | J/mol×K | 837.97 | Joback Method |
| cpg | 867.86 | J/mol×K | 867.34 | Joback Method |

# Sources

| | |
|---|---|
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U130810&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 |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **af:** | Acentric Factor |
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |