

# 9-Tetradecen-1-ol, acetate, (E)-

|                      |                                                                                                                                                            |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | (E)-9-Tetradecen-1-ol acetate<br>E-9-Tetradecen-1-yl acetate<br>E-9-Tetradecenyl acetate<br>(9E)-9-Tetradecenyl acetate<br>trans-9-Tetradecen-1-yl acetate |
| Inchi:               | InChI=1S/C16H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-16(2)17/h6-7H,3-5,8-15H2                                                                           |
| InchiKey:            | XXPBOEBNDHAAQH-VOTSOKGWSA-N                                                                                                                                |
| Formula:             | C16H30O2                                                                                                                                                   |
| SMILES:              | CCCCC=CCCCCCCCCOC(C)=O                                                                                                                                     |
| Mol. weight [g/mol]: | 254.41                                                                                                                                                     |
| CAS:                 | 23192-82-7                                                                                                                                                 |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -69.86  | kJ/mol  | Joback Method  |
| hf            | -501.15 | kJ/mol  | Joback Method  |
| hfus          | 40.18   | kJ/mol  | Joback Method  |
| hvap          | 89.60   | kJ/mol  | NIST Webbook   |
| log10ws       | -5.24   |         | Crippen Method |
| logp          | 5.027   |         | Crippen Method |
| mcvol         | 239.440 | ml/mol  | McGowan Method |
| pc            | 1417.57 | kPa     | Joback Method  |
| rinpol        | 1801.00 |         | NIST Webbook   |
| rinpol        | 1801.00 |         | NIST Webbook   |
| ripol         | 2116.00 |         | NIST Webbook   |
| tb            | 645.93  | K       | Joback Method  |
| tc            | 818.34  | K       | Joback Method  |
| tf            | 337.16  | K       | Joback Method  |
| vc            | 0.935   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

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

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 672.59    | J/mol×K | 674.67 | Joback Method |
| cpg   | 689.29    | J/mol×K | 703.40 | Joback Method |
| cpg   | 705.23    | J/mol×K | 732.14 | Joback Method |
| cpg   | 720.44    | J/mol×K | 760.87 | Joback Method |
| cpg   | 734.94    | J/mol×K | 789.61 | Joback Method |
| cpg   | 748.76    | J/mol×K | 818.34 | Joback Method |
| dvisc | 0.0022449 | Pa×s    | 337.16 | Joback Method |
| dvisc | 0.0009605 | Pa×s    | 388.62 | Joback Method |
| dvisc | 0.0005012 | Pa×s    | 440.08 | Joback Method |
| dvisc | 0.0002997 | Pa×s    | 491.55 | Joback Method |
| dvisc | 0.0001976 | Pa×s    | 543.01 | Joback Method |
| dvisc | 0.0001400 | Pa×s    | 594.47 | Joback Method |
| dvisc | 0.0001048 | Pa×s    | 645.93 | Joback Method |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C23192827&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23192827&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |

**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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