

# 1-Hexadecanol, 14-chloro, acetate

|                      |                                                                                 |
|----------------------|---------------------------------------------------------------------------------|
| Other names:         | 14-Chlorohexadecyl acetate                                                      |
| Inchi:               | InChI=1S/C18H35ClO2/c1-3-18(19)15-13-11-9-7-5-4-6-8-10-12-14-16-21-17(20)/h18H, |
| InchiKey:            | UAXSCUVDZMUXCU-UHFFFAOYSA-N                                                     |
| Formula:             | C18H35ClO2                                                                      |
| SMILES:              | CCC(Cl)CCCCCCCCCCCCCOC(C)=O                                                     |
| Mol. weight [g/mol]: | 318.92                                                                          |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -147.61 | kJ/mol  | Joback Method  |
| hf            | -680.67 | kJ/mol  | Joback Method  |
| hfus          | 45.84   | kJ/mol  | Joback Method  |
| hvap          | 68.81   | kJ/mol  | Joback Method  |
| log10ws       | -6.48   |         | Crippen Method |
| logp          | 6.248   |         | Crippen Method |
| mcvol         | 284.160 | ml/mol  | McGowan Method |
| pc            | 1165.63 | kPa     | Joback Method  |
| tb            | 724.52  | K       | Joback Method  |
| tc            | 899.87  | K       | Joback Method  |
| tf            | 379.70  | K       | Joback Method  |
| vc            | 1.111   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 825.77    | J/mol×K | 724.52          | Joback Method |
| cpg           | 843.94    | J/mol×K | 753.74          | Joback Method |
| cpg           | 861.23    | J/mol×K | 782.97          | Joback Method |
| cpg           | 877.67    | J/mol×K | 812.19          | Joback Method |
| cpg           | 893.27    | J/mol×K | 841.42          | Joback Method |
| cpg           | 908.06    | J/mol×K | 870.64          | Joback Method |
| cpg           | 922.05    | J/mol×K | 899.87          | Joback Method |
| dvisc         | 0.0019853 | Pa×s    | 379.70          | Joback Method |
| dvisc         | 0.0008119 | Pa×s    | 437.17          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0004087 | Pa×s | 494.64 | Joback Method |
| dvisc | 0.0002373 | Pa×s | 552.11 | Joback Method |
| dvisc | 0.0001527 | Pa×s | 609.58 | Joback Method |
| dvisc | 0.0001060 | Pa×s | 667.05 | Joback Method |
| dvisc | 0.0000780 | Pa×s | 724.52 | Joback Method |

## Sources

|                        |                                                                                                                                         |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                   |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R33238&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R33238&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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