

# (Z)-2-(E)-13-Octadecadien-1-ol acetate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H36O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-20(2)21/h6-7,

NWRSOYAGXTXEMK-NEOCR XKBSA-N

C20H36O2

CCCCC=CCCCCCCCCCC=CCOC(C)=O

308.50

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 44.04   | kJ/mol  | Joback Method  |
| hf            | -466.49 | kJ/mol  | Joback Method  |
| hfus          | 50.75   | kJ/mol  | Joback Method  |
| hvap          | 69.19   | kJ/mol  | Joback Method  |
| log10ws       | -6.76   |         | Crippen Method |
| logp          | 6.363   |         | Crippen Method |
| mcvol         | 291.500 | ml/mol  | McGowan Method |
| pc            | 1120.05 | kPa     | Joback Method  |
| rinpol        | 2078.00 |         | NIST Webbook   |
| rinpol        | 2078.00 |         | NIST Webbook   |
| ripol         | 2056.00 |         | NIST Webbook   |
| tb            | 741.61  | K       | Joback Method  |
| tc            | 919.70  | K       | Joback Method  |
| tf            | 377.16  | K       | Joback Method  |
| vc            | 1.139   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 862.13 | J/mol×K | 741.61          | Joback Method |
| cpg           | 946.80 | J/mol×K | 890.02          | Joback Method |
| cpg           | 931.49 | J/mol×K | 860.34          | Joback Method |
| cpg           | 915.41 | J/mol×K | 830.65          | Joback Method |
| cpg           | 898.51 | J/mol×K | 800.97          | Joback Method |
| cpg           | 880.77 | J/mol×K | 771.29          | Joback Method |
| cpg           | 961.38 | J/mol×K | 919.70          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000550 | Pa×s | 741.61 | Joback Method |
| dvisc | 0.0000744 | Pa×s | 680.87 | Joback Method |
| dvisc | 0.0001068 | Pa×s | 620.13 | Joback Method |
| dvisc | 0.0001659 | Pa×s | 559.38 | Joback Method |
| dvisc | 0.0002868 | Pa×s | 498.64 | Joback Method |
| dvisc | 0.0005772 | Pa×s | 437.90 | Joback Method |
| dvisc | 0.0014552 | Pa×s | 377.16 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                                 |
| <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=R571825&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R571825&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                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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