# E-3-OCTADECEN-1-OL ACETATE

**Inchi:** InChI=1S/C20H38O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-20(2)21/h16-1
**InchiKey:** KPESFCKQDRGZJA-WUKNDPDISA-N
**Formula:** C20H38O2
**SMILES:** CCCCCCCCCCCCCC/C=C/CCOC(C)=O
**Mol. weight [g/mol]:** 310.52

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.8749 | | Cheméo Relay (1.0) |
| gf | -36.18 | kJ/mol | Joback Method |
| hf | -685.53 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 50.54 | kJ/mol | Joback Method |
| hvap | 105.11 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.11 | eV | Cheméo Relay (1.0) |
| log10ws | -6.76 | | Cheméo Relay (1.0) |
| logp | 6.587 | | Crippen Method |
| mcvol | 295.800 | ml/mol | McGowan Method |
| pc | 1082.06 | kPa | Joback Method |
| rinpol | 2192.00 | | NIST Webbook |
| ripol | 2027.00 | | NIST Webbook |
| tb | 593.12 | K | Cheméo Relay (1.0) |
| tc | 776.07 | K | Cheméo Relay (1.0) |
| tf | 286.64 | K | Cheméo Relay (1.0) |
| vc | 1.124 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 885.45 | J/mol×K | 737.45 | Joback Method |
| cpg | 987.32 | J/mol×K | 911.93 | Joback Method |
| cpg | 972.40 | J/mol×K | 882.85 | Joback Method |
| cpg | 956.69 | J/mol×K | 853.77 | Joback Method |
| cpg | 940.17 | J/mol×K | 824.69 | Joback Method |
| cpg | 922.81 | J/mol×K | 795.61 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 904.58 | J/mol×K | 766.53 | Joback Method |
| dvisc | 0.0001891 | Pa×s | 559.85 | Joback Method |
| dvisc | 0.0000635 | Pa×s | 737.45 | Joback Method |
| dvisc | 0.0000857 | Pa×s | 678.25 | Joback Method |
| dvisc | 0.0001226 | Pa×s | 619.05 | Joback Method |
| dvisc | 0.0015546 | Pa×s | 382.24 | Joback Method |
| dvisc | 0.0003233 | Pa×s | 500.64 | Joback Method |
| dvisc | 0.0006381 | Pa×s | 441.44 | Joback Method |

# Sources

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U130944&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

**Cheméo Relay (1.0):**

# 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