

(Z)-3-Hexadecenyl acetate

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| Inchi: | InChI=1S/C18H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-18(2)19/h14-15H,3- |
| InchiKey: | NJOIVGUNIXAPULH-PFONDFGASA-N |
| Formula: | C18H34O2 |
| SMILES: | CCCCCCCCCCCC=CCOC(C)=O |
| Mol. weight [g/mol]: | 282.46 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -53.02 | kJ/mol | Joback Method |
| hf | -542.43 | kJ/mol | Joback Method |
| hfus | 45.36 | kJ/mol | Joback Method |
| hvap | 64.78 | kJ/mol | Joback Method |
| log10ws | -6.07 | | Crippen Method |
| logp | 5.807 | | Crippen Method |
| mvol | 267.620 | ml/mol | McGowan Method |
| pc | 1232.88 | kPa | Joback Method |
| ripol | 1994.00 | | NIST Webbook |
| ripol | 2310.00 | | NIST Webbook |
| tb | 691.69 | K | Joback Method |
| tc | 864.16 | K | Joback Method |
| tf | 359.70 | K | Joback Method |
| vc | 1.048 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 768.00 | J/molxK | 691.69 | Joback Method |
| cpg | 786.32 | J/molxK | 720.43 | Joback Method |
| cpg | 803.81 | J/molxK | 749.18 | Joback Method |
| cpg | 820.48 | J/molxK | 777.92 | Joback Method |
| cpg | 836.37 | J/molxK | 806.67 | Joback Method |
| cpg | 851.50 | J/molxK | 835.41 | Joback Method |
| cpg | 865.91 | J/molxK | 864.16 | Joback Method |
| dvisc | 0.0018910 | Paxs | 359.70 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0007915 | Paxs | 415.03 | Joback Method |
| dvisc | 0.0004066 | Paxs | 470.36 | Joback Method |
| dvisc | 0.0002403 | Paxs | 525.70 | Joback Method |
| dvisc | 0.0001570 | Paxs | 581.03 | Joback Method |
| dvisc | 0.0001105 | Paxs | 636.36 | Joback Method |
| dvisc | 0.0000822 | Paxs | 691.69 | Joback Method |

Sources

| | |
|------------------------|---|
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R86926&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|---|
| 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 |
| 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 |

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<https://www.chemeo.com/cid/23-490-2/Z-3-Hexadecenyl-acetate.pdf>

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