

# 3-Heptadecene, (z)-

|                      |                                                                                    |
|----------------------|------------------------------------------------------------------------------------|
| Other names:         | cis-3-Heptadecene<br>(Z)-3-Heptadecene                                             |
| Inchi:               | InChI=1S/C17H34/c1-3-5-7-9-11-13-15-17-16-14-12-10-8-6-4-2/h5,7H,3-4,6,8-17H2,1-2H |
| InchiKey:            | YICJXYRVTBRLKS-ALCCZGGFSA-N                                                        |
| Formula:             | C17H34                                                                             |
| SMILES:              | CC/C=C\CCCCCCCCCCCCC                                                               |
| Mol. weight [g/mol]: | 238.46                                                                             |

## Physical Properties

| Property code | Value   | Unit    | Source             |
|---------------|---------|---------|--------------------|
| af            | 0.6865  |         | Cheméo Relay (1.0) |
| gf            | 172.48  | kJ/mol  | Joback Method      |
| hf            | -296.67 | kJ/mol  | Cheméo Relay (1.0) |
| hfus          | 39.99   | kJ/mol  | Joback Method      |
| hvap          | 81.90   | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 9.01    | eV      | Cheméo Relay (1.0) |
| log10ws       | -7.31   |         | Cheméo Relay (1.0) |
| logp          | 6.654   |         | Crippen Method     |
| mcvol         | 246.090 | ml/mol  | McGowan Method     |
| pc            | 1277.33 | kPa     | Joback Method      |
| rinpol        | 1692.00 |         | NIST Webbook       |
| rinpol        | 1687.40 |         | NIST Webbook       |
| rinpol        | 1688.70 |         | NIST Webbook       |
| ripol         | 1723.00 |         | NIST Webbook       |
| ripol         | 1756.00 |         | NIST Webbook       |
| ripol         | 1722.60 |         | NIST Webbook       |
| tb            | 548.38  | K       | Cheméo Relay (1.0) |
| tc            | 722.34  | K       | Cheméo Relay (1.0) |
| tf            | 251.73  | K       | Cheméo Relay (1.0) |
| vc            | 0.964   | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|------|-----------------|--------|
|---------------|-------|------|-----------------|--------|

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 648.17    | J/mol×K | 592.52 | Joback Method |
| cpg   | 667.50    | J/mol×K | 619.83 | Joback Method |
| cpg   | 686.02    | J/mol×K | 647.13 | Joback Method |
| cpg   | 703.76    | J/mol×K | 674.44 | Joback Method |
| cpg   | 720.76    | J/mol×K | 701.74 | Joback Method |
| cpg   | 737.03    | J/mol×K | 729.05 | Joback Method |
| cpg   | 752.62    | J/mol×K | 756.35 | Joback Method |
| dvisc | 0.0044937 | Pa×s    | 276.27 | Joback Method |
| dvisc | 0.0015040 | Pa×s    | 328.98 | Joback Method |
| dvisc | 0.0006810 | Pa×s    | 381.69 | Joback Method |
| dvisc | 0.0003738 | Pa×s    | 434.39 | Joback Method |
| dvisc | 0.0002336 | Pa×s    | 487.10 | Joback Method |
| dvisc | 0.0001600 | Pa×s    | 539.81 | Joback Method |
| dvisc | 0.0001172 | Pa×s    | 592.52 | Joback Method |

## Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U141673&Units=SI>

Joback Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                 |
| <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>ie:</b>      | Ionization energy                               |
| <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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