

# 2-Hexen-1-ol, (Z)-

|                      |                                                                                                                                                        |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | (Z)-2-Hexenol<br>(Z)-Hex-2-en-1-ol<br>(Z)-Hex-2-ene-1-ol<br>(Z)-Hex-2-enol<br>Z-2-Hexen-1-ol<br>cis-2-Hexen-1-ol<br>cis-2-Hexenol<br>cis-hex-2-en-1-ol |
| Inchi:               | InChI=1S/C6H12O/c1-2-3-4-5-6-7/h4-5,7H,2-3,6H2,1H3/b5-4-                                                                                               |
| InchiKey:            | ZCHHRLHTBGRGOT-PLNGDYQASA-N                                                                                                                            |
| Formula:             | C6H12O                                                                                                                                                 |
| SMILES:              | CCCC=CCO                                                                                                                                               |
| Mol. weight [g/mol]: | 100.16                                                                                                                                                 |
| CAS:                 | 928-94-9                                                                                                                                               |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -56.96  | kJ/mol | Joback Method  |
| hf            | -202.18 | kJ/mol | Joback Method  |
| hfus          | 15.59   | kJ/mol | Joback Method  |
| hvap          | 45.59   | kJ/mol | Joback Method  |
| log10ws       | -1.45   |        | Crippen Method |
| logp          | 1.335   |        | Crippen Method |
| mcvol         | 96.970  | ml/mol | McGowan Method |
| pc            | 3673.09 | kPa    | Joback Method  |
| rinpol        | 865.00  |        | NIST Webbook   |
| rinpol        | 856.00  |        | NIST Webbook   |
| rinpol        | 847.00  |        | NIST Webbook   |
| rinpol        | 868.00  |        | NIST Webbook   |
| rinpol        | 827.00  |        | NIST Webbook   |
| rinpol        | 856.00  |        | NIST Webbook   |
| rinpol        | 856.00  |        | NIST Webbook   |
| rinpol        | 855.00  |        | NIST Webbook   |
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| rinpol        | 855.00  |        | NIST Webbook   |
| rinpol        | 855.00  |        | NIST Webbook   |
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| rinpol | 837.00  | NIST Webbook |
| rinpol | 845.00  | NIST Webbook |
| rinpol | 846.00  | NIST Webbook |
| rinpol | 866.00  | NIST Webbook |
| rinpol | 872.00  | NIST Webbook |
| rinpol | 870.00  | NIST Webbook |
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| rinpol | 875.00  | NIST Webbook |
| rinpol | 854.00  | NIST Webbook |
| rinpol | 868.00  | NIST Webbook |
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| ripol  | 1405.00 | NIST Webbook |
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| ripol  | 1405.00 | NIST Webbook |
| ripol  | 1380.00 | NIST Webbook |
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| ripol  | 1389.00 | NIST Webbook |
| ripol  | 1402.00 | NIST Webbook |
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| ripol  | 1398.00 | NIST Webbook |
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| ripol  | 1419.00 | NIST Webbook |
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|-------|---------|---------|---------------|
| ripol | 1401.00 |         | NIST Webbook  |
| ripol | 1397.00 |         | NIST Webbook  |
| ripol | 1420.00 |         | NIST Webbook  |
| ripol | 1417.00 |         | NIST Webbook  |
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| ripol | 1407.00 |         | NIST Webbook  |
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| ripol | 1416.00 |         | NIST Webbook  |
| ripol | 1416.00 |         | NIST Webbook  |
| ripol | 1368.00 |         | NIST Webbook  |
| ripol | 1413.00 |         | NIST Webbook  |
| tb    | 430.20  | K       | NIST Webbook  |
| tc    | 601.76  | K       | Joback Method |
| tf    | 213.12  | K       | Joback Method |
| vc    | 0.370   | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 191.78    | J/mol×K | 433.02          | Joback Method |
| cpg           | 233.69    | J/mol×K | 573.64          | Joback Method |
| cpg           | 226.05    | J/mol×K | 545.51          | Joback Method |
| cpg           | 218.06    | J/mol×K | 517.39          | Joback Method |
| cpg           | 209.69    | J/mol×K | 489.27          | Joback Method |
| cpg           | 200.94    | J/mol×K | 461.14          | Joback Method |
| cpg           | 240.99    | J/mol×K | 601.76          | Joback Method |
| dvisc         | 0.0002006 | Pa×s    | 433.02          | Joback Method |
| dvisc         | 0.0003473 | Pa×s    | 396.37          | Joback Method |
| dvisc         | 0.0006726 | Pa×s    | 359.72          | Joback Method |
| dvisc         | 0.0015133 | Pa×s    | 323.07          | Joback Method |
| dvisc         | 0.0041899 | Pa×s    | 286.42          | Joback Method |
| dvisc         | 0.0156415 | Pa×s    | 249.77          | Joback Method |
| dvisc         | 0.0918576 | Pa×s    | 213.12          | Joback Method |

# Pressure Dependent Properties

| Property code | Value         | Unit | Pressure [kPa] | Source       |
|---------------|---------------|------|----------------|--------------|
| tbrp          | 345.00 ± 1.00 | K    | 2.40           | NIST Webbook |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.60167e+01                   |
| Coeff. B                    | -4.20816e+03                  |
| Coeff. C                    | -6.10100e+01                  |
| Temperature range (K), min. | 328.55                        |
| Temperature range (K), max. | 454.10                        |

## Sources

|                                      |                                                                                                                                                                                         |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C928949&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C928949&amp;Units=SI</a>                                               |
| The Yaws Handbook of Vapor Pressure: | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |
| Crippen Method:                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                                                               |
| Crippen Method:                      | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                                                                       |
| Joback Method:                       | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                   |
| McGowan Method:                      | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |

## Legend

|        |                                              |
|--------|----------------------------------------------|
| cpg:   | Ideal gas heat capacity                      |
| dvisc: | Dynamic viscosity                            |
| gf:    | Standard Gibbs free energy of formation      |
| hf:    | 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>pvap:</b>    | Vapor pressure                                  |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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