

# 6-Dodecenol

|                      |                                                                               |
|----------------------|-------------------------------------------------------------------------------|
| Other names:         | (E) 6-dodecen-1-ol<br>6-Dodecen-1-ol                                          |
| Inchi:               | InChI=1S/C12H24O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h6-7,13H,2-5,8-12H2,1H3/b7-6+ |
| InchiKey:            | IENBWMQKVZLORT-VOTSOKGWSA-N                                                   |
| Formula:             | C12H24O                                                                       |
| SMILES:              | CCCCC=CCCCCO                                                                  |
| Mol. weight [g/mol]: | 184.32                                                                        |
| CAS:                 | 52957-14-9                                                                    |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -6.44   | kJ/mol  | Joback Method  |
| hf            | -326.02 | kJ/mol  | Joback Method  |
| hfus          | 31.13   | kJ/mol  | Joback Method  |
| hvap          | 90.70   | kJ/mol  | NIST Webbook   |
| log10ws       | -3.96   |         | Crippen Method |
| logp          | 3.676   |         | Crippen Method |
| mcvol         | 181.510 | ml/mol  | McGowan Method |
| pc            | 2018.13 | kPa     | Joback Method  |
| tb            | 570.30  | K       | Joback Method  |
| tc            | 733.56  | K       | Joback Method  |
| tf            | 280.74  | K       | Joback Method  |
| vc            | 0.707   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 459.51 | J/mol×K | 570.30          | Joback Method |
| cpg           | 524.90 | J/mol×K | 706.35          | Joback Method |
| cpg           | 512.93 | J/mol×K | 679.14          | Joback Method |
| cpg           | 500.43 | J/mol×K | 651.93          | Joback Method |
| cpg           | 487.37 | J/mol×K | 624.72          | Joback Method |
| cpg           | 473.74 | J/mol×K | 597.51          | Joback Method |
| cpg           | 536.36 | J/mol×K | 733.56          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000721 | Pa×s | 570.30 | Joback Method |
| dvisc | 0.0001199 | Pa×s | 522.04 | Joback Method |
| dvisc | 0.0002211 | Pa×s | 473.78 | Joback Method |
| dvisc | 0.0004685 | Pa×s | 425.52 | Joback Method |
| dvisc | 0.0012026 | Pa×s | 377.26 | Joback Method |
| dvisc | 0.0040712 | Pa×s | 329.00 | Joback Method |
| dvisc | 0.0209597 | Pa×s | 280.74 | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.44974e+01                   |
| Coeff. B                    | -4.60063e+03                  |
| Coeff. C                    | -9.07560e+01                  |
| Temperature range (K), min. | 414.52                        |
| Temperature range (K), max. | 591.59                        |

## Sources

|                                      |                                                                                                                                                                                         |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method:                      | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |
| NIST Webbook:                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C52957149&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52957149&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>                                                                                   |

## 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>h<sub>vap</sub>:</b>               | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>w<sub>s</sub>:</b> | Log10 of Water solubility in mol/l              |
| <b>log<sub>p</sub>:</b>               | Octanol/Water partition coefficient             |
| <b>mc<sub>vol</sub>:</b>              | McGowan's characteristic volume                 |
| <b>p<sub>c</sub>:</b>                 | Critical Pressure                               |
| <b>p<sub>vap</sub>:</b>               | Vapor pressure                                  |
| <b>t<sub>b</sub>:</b>                 | Normal Boiling Point Temperature                |
| <b>t<sub>c</sub>:</b>                 | Critical Temperature                            |
| <b>t<sub>f</sub>:</b>                 | Normal melting (fusion) point                   |
| <b>v<sub>c</sub>:</b>                 | Critical Volume                                 |

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