

# 9-Dodecenol, trans

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | (9E)-9-Dodecen-1-ol<br>(E)-9-Dodecenyl alcohol<br>(E)9-Dodecen-1-ol<br>9-Dodecen-1-ol<br>9-Dodecen-1-ol, (9E)-<br>9-Dodecen-1-ol, (E)-<br>9-Dodecenol, E<br>trans-9-Dodecen-1-ol |
| <b>Inchi:</b>               | InChI=1S/C12H24O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h3-4,13H,2,5-12H2,1H3/b4-3+  |
| <b>InchiKey:</b>            | GJNNIRNIXNLOJP-ONEGZZNKSA-N  |
| <b>Formula:</b>             | C12H24O  |
| <b>SMILES:</b>              | CCC=CCCCCCCCCO   |
| <b>Mol. weight [g/mol]:</b> | 184.32   |
| <b>CAS:</b>                 | 35237-62-8   |

## 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          | 91.70   | 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  |
| ripol         | 1469.00 |                      | NIST Webbook   |
| ripol         | 1470.00 |                      | NIST Webbook   |
| ripol         | 1428.00 |                      | NIST Webbook   |
| ripol         | 1470.00 |                      | NIST Webbook   |
| ripol         | 2043.00 |                      | NIST Webbook   |
| ripol         | 2013.00 |                      | NIST Webbook   |
| ripol         | 2013.00 |                      | NIST Webbook   |
| ripol         | 1994.00 |                      | NIST Webbook   |
| tb            | 570.30  | K                    | Joback Method  |
| tc            | 733.56  | K                    | Joback Method  |
| tf            | 280.74  | K                    | Joback Method  |
| vc            | 0.707   | m <sup>3</sup> /kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 459.51    | J/molxK | 570.30          | Joback Method |
| cpg           | 473.74    | J/molxK | 597.51          | Joback Method |
| cpg           | 487.37    | J/molxK | 624.72          | Joback Method |
| cpg           | 500.43    | J/molxK | 651.93          | Joback Method |
| cpg           | 512.93    | J/molxK | 679.14          | Joback Method |
| cpg           | 524.90    | J/molxK | 706.35          | Joback Method |
| cpg           | 536.36    | J/molxK | 733.56          | Joback Method |
| dvisc         | 0.0209597 | Paxs    | 280.74          | Joback Method |
| dvisc         | 0.0040712 | Paxs    | 329.00          | Joback Method |
| dvisc         | 0.0012026 | Paxs    | 377.26          | Joback Method |
| dvisc         | 0.0004685 | Paxs    | 425.52          | Joback Method |
| dvisc         | 0.0002211 | Paxs    | 473.78          | Joback Method |
| dvisc         | 0.0001199 | Paxs    | 522.04          | Joback Method |
| dvisc         | 0.0000721 | Paxs    | 570.30          | 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

The Yaws Handbook of Vapor

Pressure:  
Crippen Method:

Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>   |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C35237628&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C35237628&amp;Units=SI</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>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>mccvol:</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>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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