

# 2-Nonen-1-ol

|                      |                                                            |
|----------------------|------------------------------------------------------------|
| Other names:         | 2-Nonene-1-ol<br>Non-2-en-1-ol                             |
| Inchi:               | InChI=1S/C9H18O/c1-2-3-4-5-6-7-8-9-10/h7-8,10H,2-6,9H2,1H3 |
| InchiKey:            | NSSALFVIQPAIQK-UHFFFAOYSA-N                                |
| Formula:             | C9H18O                                                     |
| SMILES:              | CCCCCCC=CCO                                                |
| Mol. weight [g/mol]: | 142.24                                                     |
| CAS:                 | 22104-79-6                                                 |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -31.70  | kJ/mol  | Joback Method  |
| hf            | -264.10 | kJ/mol  | Joback Method  |
| hfus          | 23.36   | kJ/mol  | Joback Method  |
| hvap          | 52.27   | kJ/mol  | Joback Method  |
| log10ws       | -2.71   |         | Crippen Method |
| logp          | 2.505   |         | Crippen Method |
| mcvol         | 139.240 | ml/mol  | McGowan Method |
| pc            | 2662.52 | kPa     | Joback Method  |
| rinpol        | 1105.00 |         | NIST Webbook   |
| rinpol        | 1051.00 |         | NIST Webbook   |
| rinpol        | 1051.00 |         | NIST Webbook   |
| ripol         | 1692.00 |         | NIST Webbook   |
| ripol         | 1692.00 |         | NIST Webbook   |
| tb            | 501.66  | K       | Joback Method  |
| tc            | 667.34  | K       | Joback Method  |
| tf            | 246.93  | K       | Joback Method  |
| vc            | 0.538   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 317.11 | J/mol×K | 501.66          | Joback Method |
| cpg           | 329.17 | J/mol×K | 529.27          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 340.72    | J/mol×K | 556.89 | Joback Method |
| cpg   | 351.78    | J/mol×K | 584.50 | Joback Method |
| cpg   | 362.36    | J/mol×K | 612.11 | Joback Method |
| cpg   | 372.49    | J/mol×K | 639.73 | Joback Method |
| cpg   | 382.18    | J/mol×K | 667.34 | Joback Method |
| dvisc | 0.0432087 | Pa×s    | 246.93 | Joback Method |
| dvisc | 0.0079294 | Pa×s    | 289.38 | Joback Method |
| dvisc | 0.0022455 | Pa×s    | 331.84 | Joback Method |
| dvisc | 0.0008466 | Pa×s    | 374.30 | Joback Method |
| dvisc | 0.0003894 | Pa×s    | 416.75 | Joback Method |
| dvisc | 0.0002067 | Pa×s    | 459.21 | Joback Method |
| dvisc | 0.0001222 | Pa×s    | 501.66 | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.50585e+01                   |
| Coeff. B                    | -4.39676e+03                  |
| Coeff. C                    | -7.68560e+01                  |
| Temperature range (K), min. | 374.52                        |
| Temperature range (K), max. | 527.94                        |

## Sources

|                                             |                                                                                                                                                                                         |
|---------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <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=C22104796&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22104796&amp;Units=SI</a>                                           |
| <b>The Yaws Handbook of Vapor Pressure:</b> | <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> |
| <b>Crippen Method:</b>                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                                                               |
| <b>Crippen Method:</b>                      | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                                                                       |

## Legend

**cpg:** 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>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>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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