

# 3-Octen-2-one

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 3-Oct-3-en-2-one<br>oct-3-en-2-one                   |
| <b>Inchi:</b>               | InChI=1S/C8H14O/c1-3-4-5-6-7-8(2)9/h6-7H,3-5H2,1-2H3 |
| <b>InchiKey:</b>            | ZCFOBLITZWHNNC-UHFFFAOYSA-N                          |
| <b>Formula:</b>             | C8H14O   |
| <b>SMILES:</b>              | CCCCC=CC(C)=O  |
| <b>Mol. weight [g/mol]:</b> | 126.20   |
| <b>CAS:</b>                 | 1669-44-9  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -32.22  | kJ/mol | Joback Method  |
| hf            | -203.81 | kJ/mol | Joback Method  |
| hfus          | 18.28   | kJ/mol | Joback Method  |
| hvap          | 40.11   | kJ/mol | Joback Method  |
| log10ws       | -2.30   |        | Crippen Method |
| logp          | 2.322   |        | Crippen Method |
| mcvol         | 120.850 | ml/mol | McGowan Method |
| pc            | 2856.62 | kPa    | Joback Method  |
| rinpol        | 1053.00 |        | NIST Webbook   |
| rinpol        | 1014.00 |        | NIST Webbook   |
| rinpol        | 1043.00 |        | NIST Webbook   |
| rinpol        | 1040.00 |        | NIST Webbook   |
| rinpol        | 1040.00 |        | NIST Webbook   |
| rinpol        | 1048.00 |        | NIST Webbook   |
| rinpol        | 1037.00 |        | NIST Webbook   |
| rinpol        | 1013.00 |        | NIST Webbook   |
| rinpol        | 1023.00 |        | NIST Webbook   |
| rinpol        | 1043.00 |        | NIST Webbook   |
| rinpol        | 1038.00 |        | NIST Webbook   |
| rinpol        | 1016.00 |        | NIST Webbook   |
| rinpol        | 1046.00 |        | NIST Webbook   |
| rinpol        | 1015.00 |        | NIST Webbook   |
| rinpol        | 1018.00 |        | NIST Webbook   |
| rinpol        | 1036.00 |        | NIST Webbook   |
| rinpol        | 1042.00 |        | NIST Webbook   |
| rinpol        | 1040.00 |        | NIST Webbook   |

|       |         |                      |               |
|-------|---------|----------------------|---------------|
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| ripol | 1042.00 |                      | NIST Webbook  |
| ripol | 1037.00 |                      | NIST Webbook  |
| ripol | 1014.00 |                      | NIST Webbook  |
| ripol | 1036.00 |                      | NIST Webbook  |
| ripol | 1016.00 |                      | NIST Webbook  |
| ripol | 1043.00 |                      | NIST Webbook  |
| ripol | 1015.00 |                      | NIST Webbook  |
| ripol | 1040.00 |                      | NIST Webbook  |
| ripol | 1020.00 |                      | NIST Webbook  |
| ripol | 1019.00 |                      | NIST Webbook  |
| ripol | 1035.00 |                      | NIST Webbook  |
| ripol | 1013.00 |                      | NIST Webbook  |
| ripol | 1011.00 |                      | NIST Webbook  |
| ripol | 1013.00 |                      | NIST Webbook  |
| ripol | 1388.00 |                      | NIST Webbook  |
| ripol | 1408.00 |                      | NIST Webbook  |
| ripol | 1415.00 |                      | NIST Webbook  |
| ripol | 1408.00 |                      | NIST Webbook  |
| ripol | 1411.00 |                      | NIST Webbook  |
| ripol | 1411.00 |                      | NIST Webbook  |
| ripol | 1411.00 |                      | NIST Webbook  |
| ripol | 1440.00 |                      | NIST Webbook  |
| ripol | 1412.00 |                      | NIST Webbook  |
| ripol | 1412.00 |                      | NIST Webbook  |
| ripol | 1408.00 |                      | NIST Webbook  |
| ripol | 1414.00 |                      | NIST Webbook  |
| ripol | 1408.00 |                      | NIST Webbook  |
| ripol | 1429.00 |                      | NIST Webbook  |
| ripol | 1410.00 |                      | NIST Webbook  |
| ripol | 1363.00 |                      | NIST Webbook  |
| ripol | 1416.00 |                      | NIST Webbook  |
| ripol | 1390.00 |                      | NIST Webbook  |
| ripol | 1416.00 |                      | NIST Webbook  |
| ripol | 1416.00 |                      | NIST Webbook  |
| ripol | 1416.00 |                      | NIST Webbook  |
| ripol | 1416.00 |                      | NIST Webbook  |
| ripol | 1415.00 |                      | NIST Webbook  |
| tb    | 440.47  | K                    | Joback Method |
| tc    | 624.44  | K                    | Joback Method |
| tf    | 224.77  | K                    | Joback Method |
| vc    | 0.469   | m <sup>3</sup> /kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 239.73    | J/molxK | 440.47          | Joback Method |
| cpg           | 295.21    | J/molxK | 593.78          | Joback Method |
| cpg           | 285.17    | J/molxK | 563.12          | Joback Method |
| cpg           | 274.62    | J/molxK | 532.46          | Joback Method |
| cpg           | 263.55    | J/molxK | 501.79          | Joback Method |
| cpg           | 251.92    | J/molxK | 471.13          | Joback Method |
| cpg           | 304.76    | J/molxK | 624.44          | Joback Method |
| dvisc         | 0.0002453 | Paxs    | 440.47          | Joback Method |
| dvisc         | 0.0003179 | Paxs    | 404.52          | Joback Method |
| dvisc         | 0.0004335 | Paxs    | 368.57          | Joback Method |
| dvisc         | 0.0006321 | Paxs    | 332.62          | Joback Method |
| dvisc         | 0.0010100 | Paxs    | 296.67          | Joback Method |
| dvisc         | 0.0018362 | Paxs    | 260.72          | Joback Method |
| dvisc         | 0.0040418 | Paxs    | 224.77          | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.32660e+01                   |
| Coeff. B                    | -3.44271e+03                  |
| Coeff. C                    | -6.43930e+01                  |
| Temperature range (K), min. | 329.66                        |
| Temperature range (K), max. | 497.19                        |

## Sources

|   |   |
|---|---|
| <b>Crippen Method:</b>                      | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>   |
| <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=C1669449&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1669449&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> |

## 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>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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