

# Acetone-D6

|                      |                                                                                                                                                                                             |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | (2H6)acetone<br>(CD3)2CO<br>(D6)-2-propanone<br>2-Propanone-1,1,1,3,3,3-D6-<br>2-propanone-d6<br>Acetone, perdeutero-<br>Perdeuteroacetone<br>hexadeutero-2-propanone<br>hexadeuteroacetone |
| Inchi:               | InChI=1S/C3H6O/c1-3(2)4/h1-2H3/i1D3,2D3                                                                                                                                                     |
| InchiKey:            | CSCPPACGZOOCGX-WFGJKAKNSA-N                                                                                                                                                                 |
| Formula:             | C3D6O                                                                                                                                                                                       |
| SMILES:              | CC(C)=O                                                                                                                                                                                     |
| Mol. weight [g/mol]: | 64.12                                                                                                                                                                                       |
| CAS:                 | 666-52-4                                                                                                                                                                                    |

## Physical Properties

| Property code | Value       | Unit    | Source         |
|---------------|-------------|---------|----------------|
| ea            | 0.00 ± 0.00 | eV      | NIST Webbook   |
| gf            | -154.54     | kJ/mol  | Joback Method  |
| hf            | -217.83     | kJ/mol  | Joback Method  |
| hfus          | 5.12        | kJ/mol  | Joback Method  |
| hvap          | 29.02       | kJ/mol  | Joback Method  |
| ie            | 9.70 ± 0.01 | eV      | NIST Webbook   |
| ie            | 9.68        | eV      | NIST Webbook   |
| log10ws       | -0.36       |         | Crippen Method |
| logp          | 0.595       |         | Crippen Method |
| mcvol         | 54.700      | ml/mol  | McGowan Method |
| pc            | 4802.50     | kPa     | Joback Method  |
| tb            | 321.91      | K       | Joback Method  |
| tc            | 500.25      | K       | Joback Method  |
| tf            | 173.50      | K       | Joback Method  |
| vc            | 0.209       | m3/kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 79.50     | J/mol×K | 321.91          | Joback Method |
| cpg           | 84.99     | J/mol×K | 351.63          | Joback Method |
| cpg           | 90.30     | J/mol×K | 381.36          | Joback Method |
| cpg           | 95.42     | J/mol×K | 411.08          | Joback Method |
| cpg           | 100.37    | J/mol×K | 440.80          | Joback Method |
| cpg           | 105.14    | J/mol×K | 470.53          | Joback Method |
| cpg           | 109.74    | J/mol×K | 500.25          | Joback Method |
| dvisc         | 0.0022613 | Pa×s    | 173.50          | Joback Method |
| dvisc         | 0.0012367 | Pa×s    | 198.23          | Joback Method |
| dvisc         | 0.0007733 | Pa×s    | 222.97          | Joback Method |
| dvisc         | 0.0005311 | Pa×s    | 247.70          | Joback Method |
| dvisc         | 0.0003905 | Pa×s    | 272.44          | Joback Method |
| dvisc         | 0.0003022 | Pa×s    | 297.17          | Joback Method |
| dvisc         | 0.0002432 | Pa×s    | 321.91          | Joback Method |

## Datasets

### Speed of sound, m/s

| Temperature, K - Liquid | Pressure, kPa - Liquid | Speed of sound, m/s - Liquid |
|-------------------------|------------------------|------------------------------|
| 288.20                  | 100.00                 | 1110.6                       |
| 288.20                  | 5020.00                | 1140.7                       |
| 288.20                  | 10060.00               | 1168.2                       |
| 288.20                  | 20010.00               | 1218.6                       |
| 288.20                  | 30090.00               | 1264.4                       |
| 288.20                  | 40050.00               | 1302.9                       |
| 288.20                  | 49940.00               | 1345.4                       |
| 288.20                  | 60000.00               | 1382.2                       |
| 288.20                  | 70020.00               | 1417.2                       |
| 288.20                  | 80060.00               | 1450.1                       |
| 288.20                  | 90030.00               | 1481.9                       |
| 288.20                  | 100110.00              | 1512.5                       |
| 288.20                  | 110100.00              | 1540.4                       |

|        |           |        |
|--------|-----------|--------|
| 288.20 | 120100.00 | 1568.3 |
| 288.20 | 130120.00 | 1595.5 |
| 288.20 | 140000.00 | 1620.6 |
| 288.20 | 150150.00 | 1640.3 |
| 288.20 | 160030.00 | 1664.0 |
| 298.25 | 100.00    | 1071.6 |
| 298.25 | 5080.00   | 1103.4 |
| 298.25 | 10170.00  | 1131.8 |
| 298.25 | 20270.00  | 1183.7 |
| 298.25 | 30000.00  | 1229.6 |
| 298.25 | 40010.00  | 1272.1 |
| 298.25 | 50020.00  | 1312.0 |
| 298.25 | 60450.00  | 1350.7 |
| 298.25 | 70020.00  | 1383.8 |
| 298.25 | 80010.00  | 1416.9 |
| 298.25 | 90200.00  | 1443.5 |
| 298.25 | 100040.00 | 1478.7 |
| 298.25 | 110070.00 | 1507.6 |
| 298.25 | 120040.00 | 1535.4 |
| 298.25 | 130020.00 | 1561.1 |
| 298.25 | 140020.00 | 1586.5 |
| 298.25 | 150120.00 | 1611.2 |
| 298.25 | 159970.00 | 1634.8 |
| 308.22 | 100.00    | 1033.3 |
| 308.22 | 5040.00   | 1063.2 |
| 308.22 | 10000.00  | 1093.5 |
| 308.22 | 20090.00  | 1147.9 |
| 308.22 | 29990.00  | 1196.3 |
| 308.22 | 40040.00  | 1240.8 |
| 308.22 | 50090.00  | 1281.7 |
| 308.22 | 60060.00  | 1319.5 |
| 308.22 | 70070.00  | 1355.0 |
| 308.22 | 80090.00  | 1388.6 |
| 308.22 | 89970.00  | 1420.3 |
| 308.22 | 100070.00 | 1450.8 |
| 308.22 | 110070.00 | 1479.7 |
| 308.22 | 120060.00 | 1507.5 |
| 308.22 | 130120.00 | 1534.3 |
| 308.22 | 140080.00 | 1559.4 |
| 308.22 | 150120.00 | 1584.0 |
| 308.22 | 160000.00 | 1607.2 |
| 318.22 | 100.00    | 991.2  |
| 318.22 | 4980.00   | 1022.9 |
| 318.22 | 10070.00  | 1053.8 |

|        |           |        |
|--------|-----------|--------|
| 318.22 | 19990.00  | 1109.8 |
| 318.22 | 30040.00  | 1161.1 |
| 318.22 | 40070.00  | 1207.9 |
| 318.22 | 50060.00  | 1250.3 |
| 318.22 | 60010.00  | 1289.3 |
| 318.22 | 70120.00  | 1326.3 |
| 318.22 | 80030.00  | 1360.3 |
| 318.22 | 90090.00  | 1393.0 |
| 318.22 | 100300.00 | 1424.8 |
| 318.22 | 110120.00 | 1453.2 |
| 318.22 | 120030.00 | 1481.0 |
| 318.22 | 129970.00 | 1507.9 |
| 318.22 | 140110.00 | 1534.2 |
| 318.22 | 150060.00 | 1558.7 |
| 318.22 | 160060.00 | 1582.6 |
| 328.68 | 100.00    | 941.9  |
| 328.68 | 5090.00   | 977.6  |
| 328.68 | 10030.00  | 1009.5 |
| 328.68 | 20070.00  | 1068.8 |
| 328.68 | 30010.00  | 1121.9 |
| 328.68 | 40010.00  | 1171.1 |
| 328.68 | 50070.00  | 1215.9 |
| 328.68 | 60000.00  | 1256.7 |
| 328.68 | 70030.00  | 1294.8 |
| 328.68 | 80090.00  | 1330.4 |
| 328.68 | 90100.00  | 1364.0 |
| 328.68 | 100060.00 | 1396.1 |
| 328.68 | 110140.00 | 1426.4 |
| 328.68 | 120100.00 | 1454.7 |
| 328.68 | 130000.00 | 1481.9 |
| 328.68 | 140020.00 | 1508.4 |
| 328.68 | 150040.00 | 1533.8 |
| 328.68 | 160100.00 | 1557.9 |
| 338.72 | 100.00    | 888.6  |
| 338.72 | 5050.00   | 927.2  |
| 338.72 | 10020.00  | 962.5  |
| 338.72 | 20030.00  | 1025.1 |
| 338.72 | 30050.00  | 1081.4 |
| 338.72 | 40010.00  | 1132.6 |
| 338.72 | 49990.00  | 1179.8 |
| 338.72 | 60050.00  | 1223.2 |
| 338.72 | 70040.00  | 1262.8 |
| 338.72 | 79970.00  | 1299.3 |
| 338.72 | 90070.00  | 1334.7 |

|        |           |        |
|--------|-----------|--------|
| 338.72 | 100040.00 | 1367.5 |
| 338.72 | 110020.00 | 1398.5 |
| 338.72 | 119960.00 | 1428.5 |
| 338.72 | 130000.00 | 1456.6 |
| 338.72 | 140080.00 | 1484.3 |
| 338.72 | 150050.00 | 1510.5 |
| 338.72 | 159910.00 | 1535.5 |

Reference

<https://www.doi.org/10.1016/j.jct.2004.11.001>

## 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=C666524&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C666524&amp;Units=SI</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>                         |
| Deuterium isotope differences in 2-propanone, (CH <sub>3</sub> ) <sub>2</sub> CO/(CD <sub>3</sub> ) <sub>2</sub> CO: A high pressure sound-speed, density, and heat capacities study: | <a href="https://www.doi.org/10.1016/j.jct.2004.11.001">https://www.doi.org/10.1016/j.jct.2004.11.001</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>ea:</b>      | Electron affinity                               |
| <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>ie:</b>      | Ionization energy                               |
| <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>speedsl:</b> | Speed of sound in fluid                         |
| <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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