**S1: Supporting data**

Table S1.1 Physical properties of tritium and deuterium isotopologues in water and hydrogen\*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Property\*\* | H2O | D2O | **HDO** | H2 | D2 | **HD** | **T2O** | **HTO** | **DTO** | **T2** | **HT** | **DT** |
| *API* | 10.000 | -3.730 | **3.135** | 340.000 | 340.000 | **340.000** | **-12.929** | **0.801** | **-8.398** | **340.000** | **340.000** | **340.000** |
| *DGFORM* | -228.572 | -234.585 | **-55.715** | 0.000 | 0.000 | **-0.350** | **-56.618** | **-56.030** | **-56.456** | **0.000** | **-0.280** | **-0.396** |
| *DHFORM* | -241.818 | -249.199 | **-58.639** | 0.000 | 0.000 | **0.071** | **-60.701** | **-58.938** | **-60.120** | **0.000** | **0.160** | **0.020** |
| *DHVLB* | 40.694 | 41.447 | **40.677** | 0.214 | 1.192 | **1.044** | **41.952** | **41.199** | **41.704** | **0.332** | **1.094** | **1.292** |
| *FREEZEPT* | 273.150 | 276.960 | **1.905** | 13.950 | 18.732 | **-256.550** | **6.363** | **2.553** | **5.105** | **-251.214** | **-255.996** | **-252.792** |
| *MUP* | 1.850 | 1.780 | **1.815** | 0.000 | 0.000 | **0.000** | **1.733** | **1.803** | **1.756** | **0.000** | **0.000** | **0.000** |
| *MW* | 18.015 | 20.027 | **19.021** | 2.016 | 4.028 | **3.022** | **22.029** | **20.022** | **21.028** | **6.030** | **4.023** | **5.029** |
| *OMEGA* | 0.345 | 0.366 | **0.355** | -0.216 | -0.145 | **-0.180** | **0.380** | **0.359** | **0.373** | **-0.097** | **-0.168** | **-0.121** |
| *PC* | 22064.000 | 21671.000 | **21867.500** | 1313.000 | 1661.700 | **1484.000** | **21407.690** | **21800.690** | **21537.380** | **1895.329** | **1546.629** | **1780.258** |
| *RKTZRA* | 0.243 | 0.237 | **0.240** | 0.321 | 0.315 | **0.318** | **0.232** | **0.239** | **0.235** | **0.311** | **0.317** | **0.313** |
| *SG* | 1.000 | 1.107 | **1.054** | 0.300 | 0.300 | **0.300** | **1.179** | **1.072** | **1.144** | **0.300** | **0.300** | **0.300** |
| *TB* | 373.15 | 374.57 | **374** | 20.39 | 23.654 | **22.29** | **375.671** | **374.251** | **375.203** | 25.991 | **22.727** | **24.914** |
| *TC* | 647.096 | 643.89 | **645.644** | 33.19 | 38.35 | **36.06** | **641.892** | **645.098** | **642.95** | **41.957** | **36.797** | **40.254** |
| *VB* | 18.831 | 18.853 | **18.842** | 28.568 | 25.114 | **26.841** | **18.868** | **18.846** | **18.861** | **22.800** | **26.254** | **23.940** |
| *VC* | 55.947 | 56.300 | **56.124** | 64.147 | 60.263 | **62.000** | **56.536** | **56.184** | **56.420** | **57.661** | **61.545** | **58.942** |
| *VLSTD* | 18.050 | 18.130 | **18.045** | 53.558 | 53.558 | **53.558** | **18.184** | **18.104** | **18.157** | **53.558** | **53.558** | **53.558** |
| ZC | 0.229 | 0.228 | **0.229** | 0.305 | 0.314 | **0.312** | **0.227** | **0.228** | **0.228** | **0.320** | **0.311** | **0.317** |

\*:Property values in bold characters were added to Aspen plus data base.

\*\*: Nomenclature of properties: *API* : Standard API gravity [-], DGFORM: Free energy of formation at 298 K [kJ/mol], *DHFORM*: Enthalpy of formation at 298 K [kJ/mol], *DHVLB*: Enthalpy of vaporisation at the boiling point [kJ/mol], *FREEZEPT*: Freeze point [K], *MUP*: Dipole moment [Debye], *MW*: Molecular weight [g/mol], *OMEGA*: Pitzer acentric factor [-], *P*c [kPa], *RKTZRA*: Parameter for the Rackett liquid molar volume model [-], *SG*: Standard specific gravity at 298 K, *T*B: Boiling temperature [K], *T*c: Critical temperature [K], *V*B; Liquid molar volume at boiling point point [cm3/mol], *V*c: Critical volume [cm3/mol], *VLSTD*: Standard liquid molar volume at 298 K [cm3/mol], *Z*c: Critical compressibility factor[-]

Table S1.2 Properties of tritium and deuterium isotopologues in water and hydrogen with temperature

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Property | HDO | HD | H2O | D2O | H2 | D2 | T2O | HTO | DTO | T2 | HT | DT |
| CPIGDP (Ideal gas heat capacity) |
| *C*1 | 33.48 | 27.621 | 33.48 | 33.48 | 27.621 | 30.132 | 33.8985 | 33.48 | 33.8985 | 32.2245 | 32.2245 | 31.3875 |
| *C*2 | 27.2025 | 9.6255 | 26.784 | 27.621 | 9.6255 | 9.6255 | 28.458 | 27.621 | 28.0395 | 10.044 | 10.044 | 9.6255 |
| *C*3 | 10763.4 | 10320.21 | 10924.94 | 10449.95 | 10320.21 | 10525.28 | 10131.89 | 10606.88 | 10288.4 | 10662.54 | 10662.54 | 10595.2 |
| *C*4 | 11.2995 | 3.7665 | 8.7885 | 15.903 | 3.7665 | -2.9295 | 20.5065 | 13.8105 | 18.414 | -7.1145 | -7.1145 | -5.022 |
| *C*5 | 1160.3 | 567.6 | 1169.0 | 1143.5 | 567.6 | 368.0 | 1126.4 | 1151.9 | 1134.8 | 234.3 | 234.3 | 300.1 |
| *C*6 | -173.2 | -23.2 | -173.2 | -173.2 | -23.2 | -173.2 | -173.2 | -173.2 | -173.2 | -273.7 | -273.7 | -224.2 |
| *C*7 | 3267.1 | 1226.9 | 2000.0 | 5726.9 | 1226.9 | 1226.9 | 8223.8 | 4497.0 | 6994.0 | 1226.9 | 1226.9 | 1226.9 |
| DHVLDP (Heat of vaporisation)  |
| *C*1 | 59.5107 | 1.0881 | 56.5812 | 65.16045 | 1.0044 | 1.1718 | 70.8939 | 62.31465 | 68.0481 | 1.29735 | 1.12995 | 1.21365 |
| *C*2 | 0.74 | 0.36 | 0.61 | 0.98 | 0.70 | -0.31 | 1.22 | 0.86 | 1.10 | -0.99 | 0.02 | -0.65 |
| *C*3 | -0.79 | -1.10 | -0.63 | -1.11 | -1.82 | 0.28 | -1.44 | -0.95 | -1.28 | 1.69 | -0.41 | 1.00 |
| *C*4 | 0.45 | 1.07 | 0.40 | 0.56 | 1.45 | 0.35 | 0.67 | 0.51 | 0.62 | -0.39 | 0.71 | -0.03 |
| *C*5 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| *C*6 | 1.31 | -257.58 | 0.01 | 3.82 | -259.20 | -254.42 | 6.37 | 2.56 | 5.12 | -251.22 | -256.00 | -252.80 |
| *C*7 | 372.86 | -238.21 | 373.95 | 370.74 | -239.96 | -234.80 | 368.59 | 371.80 | 369.65 | -231.34 | -236.50 | -233.05 |
| DNLDIP (DIPPR liquid density)  |
| *C*1 | 0.4844 | 272.6596 | 0.4877 | 0.4781 | 412.5610 | 1.0868 | 0.4716 | 0.4812 | 0.4748 | 1.0868 | 136.8732 | 1.0868 |
| *C*2 | 0.0014 | 4.2176 | 0.0015 | 0.0011 | 6.3903 | 0.0000 | 0.0009 | 0.0012 | 0.0010 | 0.0000 | 2.1088 | 0.0000 |
| *C*3 | 0.0000 | 0.0243 | 0.0000 | 0.0000 | 0.0368 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0122 | 0.0000 |
| *C*4 | 0.0000 | 0.0001 | 0.0000 | 0.0000 | 0.0001 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| *C*5 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| *C*6 | -0.2518 | -257.0070 | 0.0100 | -0.7600 | -259.2000 | -252.7500 | -1.2759 | -0.5059 | -1.0218 | -252.7500 | -254.8785 | -252.7500 |
| *C*7 | 358.37 | -245.754 | 360 | 355.2 | -242.15 | -252.75 | 351.984 | 356.784 | 353.568 | -252.75 | -249.252 | -252.75 |
| KLDIP (DIPPR liquid thermal conductivity)  |
| *C*1 | 0.58125 | 317.0138 | 0.58125 | 0.58125 | 479.6475 | 1.27875 | 0.58125 | 0.58125 | 0.58125 | 1.27875 | 159.1463 | 1.27875 |
| *C*2 | 0.0 | 4.8825 | 0 | 0 | 7.44 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 2.44125 | 0 |
| *C*3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| *C*4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| *C*5 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| *C*6 | -0.3 | -257.0 | 0.0 | -0.8 | -259.2 | -252.8 | -1.3 | -0.5 | -1.0 | -252.8 | -254.9 | -252.8 |
| *C*7 | 358.4 | -245.8 | 360.0 | 355.2 | -242.2 | -252.8 | 352.0 | 356.8 | 353.6 | -252.8 | -249.3 | -252.8 |

|  |
| --- |
| KVDIP (DIPPR vapour thermal conductivity)  |
| *C*1 | 5.73E-06 | 0.001.85 | 0.0000062 | 0.0000048 | 0.0026 | 0.00028 | 0.0000039 | 0.0000052 | 0.0000043 | -0.0013 | 0.0010 | -5.20E-04 |
| *C*2 | 1.412464 | 0.827548 | 1.3973 | 1.4419 | 0.7452 | 0.9874 | 1.471782 | 1.427182 | 1.457064 | 1.149674 | 0.90747 | 1.069748 |
| *C*3 | 0 | -60.2534 | 0 | 0 | 12 | -200.51 | 0 | 0 | 0 | -342.892 | -130.382 | -272.7634 |
| *C*4 | 0 | 7414.38 | 0 | 0 | 0 | 21807 | 0 | 0 | 0 | 36417.69 | 14610.7 | 29221.38 |
| *C*5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| *C*6 | 1.2952 | -179.359 | 0.01 | 3.79 | -251.15 | -40 | 6.3226 | 2.5426 | 5.0752 | 101.4705 | -109.68 | 31.791 |
| *C*7 | 775.129 | 1292.85 | 800 | 726.85 | 1326.85 | 1226.85 | 677.8395 | 750.9895 | 701.979 | 1159.85 | 1259.85 | 1192.85 |
| MULDIP (DIPPR liquid viscosity)  |
| *C*1 | -140.0 | -3.1 | -45.9 | -140.2 | -4.8 | 0.0 | -140.0 | -140.0 | -140.0 | 3.2 | -1.6 | 1.6 |
| *C*2 | 7440.0 | 16.3 | 3703.6 | 7435.6 | 24.7 | 0.0 | 7440.0 | 7440.0 | 7440.0 | -16.5 | 8.2 | -8.4 |
| *C*3 | 20.5 | -0.2 | 5.9 | 20.5 | -0.3 | 0.0 | 20.5 | 20.5 | 20.5 | 0.2 | -0.1 | 0.1 |
| *C*4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| *C*5 | 2.0 | 6.6 | 10.0 | 2.0 | 10.0 | 0.0 | 2.0 | 2.0 | 2.0 | 10.0 | 10.0 | 10.0 |
| *C*6 | 3.8 | -259.2 | 0.0 | 3.8 | -259.2 | -252.8 | 3.8 | 3.8 | 3.8 | -259.2 | -259.2 | -259.2 |
| *C*7 | 365.0 | -240.2 | 373.0 | 365.0 | -240.2 | -252.8 | 365.0 | 365.0 | 365.0 | -240.2 | -240.2 | -240.2 |
| MUVDIP (DIPPR vapour viscosity)  |
| *C*1 | 0.0000175 | 0.000204 | 0.0000171 | 0.0000182 | 0.00018 | 0.00025 | 0.0000189 | 0.0000178 | 0.0000185 | 0.00025 | 0.00023 | 0.00025 |
| *C*2 | 1.113036 | 0.685952 | 1.1146 | 1.11 | 0.685 | 0.6878 | 1.106918 | 1.111518 | 1.108436 | 0.6878 | 0.68688 | 0.6878 |
| *C*3 | 0 | -0.18669 | 0 | 0 | -0.59 | 0.5962 | 0 | 0 | 0 | 0.5962 | 0.20475 | 0.5962 |
| *C*4 | 0 | 92.4 | 0 | 0 | 140 | 0 | 0 | 0 | 0 | 0 | 46.2 | 0 |
| *C*5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| *C*6 | 1.2952 | -243.543 | 0.01 | 3.79 | -259.2 | -213.15 | 6.3226 | 2.5426 | 5.0752 | -213.15 | -228.347 | -213.15 |
| *C*7 | 775.129 | 1870.05 | 800 | 726.85 | 2726.85 | 206.85 | 677.8395 | 750.9895 | 701.979 | 206.85 | 1038.45 | 206.85 |
| PLXANT (Extended Antoine equation for vapour pressure)  |
| *C*1 | 64 | 6 | 62 | 67 | 6 | 7 | 70 | 65 | 69 | 7 | 6 | 7 |
| *C*2 | -7375 | -138 | -7258 | -7601 | -113 | -159 | -7831 | -7488 | -7718 | -185 | -148 | -171 |
| *C*3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| *C*4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| *C*5 | -8 | 0 | -7 | -8 | 0 | 0 | -8 | -8 | -8 | 0 | 0 | 0 |
| *C*6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| *C*7 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| *C*8 | -5 | -269 | 0 | -15 | -269 | -269 | -26 | -10 | -21 | -269 | -269 | -269 |
| *C*9 | 373 | -235 | 374 | 371 | -235 | -235 | 369 | 372 | 370 | -235 | -235 | -235 |

 

 



Fig. S1 Deuterium and tritium isotopologue properties in both hydrogen gas and water phases. (a-d) Changes with temperature, (e) Extension of deuterium isotopologue properties to analogous tritium isotopologues: (e1) H2O isotopologues, (e2) H2 isotopologues