**D3.1. Table 3.** Boiling temperatures at different pressures in °C

| Substance | Formula | Vapor pressure in mbar | | | | | | | | | | Equation (7) | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 5 | 10 | 50 | 100 | 250 | 500 | 1,000 | 2,000 | 5,000 | 10,000 | *A* | *B* | *C* | *D* |
| **Elements** | | | | | | | | | | | | | | | |
| xenon | Xe | | | | | | | −108.3 | −95.3 | −74.2 | −54.5 | −6.00659 | 1.37325 | −0.77703 | −1.22529 |
| Krypton | Kr | | | | | | | −153.6 | −144.0 | −128.5 | −114.0 | −5.98396 | 1.34334 | −0.66521 | −1.30012 |
| Argon | Ar | | | | | | | −186.0 | −178.9 | −167.4 | −156.6 | −5.92801 | 1.21982 | −0.53967 | −1.52312 |
| Neon | Ne | | | | | | −248.2 | −246.1 | −243.6 | −239.5 | −235.6 | −5.74238 | 1.08860 | −0.05896 | −1.19851 |
| Helium | He | | | −271.0 | −270.7 | −270.1 | −269.6 | −268.9 | −268.1 | | | −4.06856 | 1.04379 | 1.11594 | 0.08835 |
| Air | | | | | | −204.8 | −200.0 | −194.4 | −187.8 | −177.0 | −167.0 | −5.35069 | −0.21537 | 0.93623 | −3.02641 |
| Hydrogen | $H_2$ | | | | −258.5 | −256.6 | −254.9 | −252.8 | −250.3 | −246.0 | −241.8 | −4.83622 | 0.94200 | 0.76650 | −0.47071 |
| Nitrogen | $N_2$ | | | | | −206.0 | −201.3 | −195.9 | −189.5 | −179.2 | −169.4 | −6.12498 | 1.26499 | −0.76765 | −1.78173 |
| Oxygen | $O_2$ | −214.6 | −211.9 | −204.4 | −200.5 | −194.5 | −189.2 | −183.1 | −175.9 | −164.3 | −153.5 | −6.05148 | 1.23506 | −0.62883 | −1.61288 |
| Sulfur | S | 211.7 | 232.1 | 287.9 | 316.6 | 360.3 | 398.8 | 443.3 | 495.5 | 579.7 | 657.9 | −15.68872 | 19.60608 | −12.56687 | 1.67046 |
| Fluorine | $F_2$ | −217.2 | −214.7 | −207.8 | −204.2 | −198.7 | −193.8 | −188.2 | −181.7 | −171.2 | −161.4 | −6.27045 | 1.53939 | −1.25605 | −1.27235 |
| Chlorine | $Cl_2$ | | | −85.8 | −76.2 | −61.7 | −48.9 | −34.3 | −17.4 | 9.6 | 34.5 | −6.43911 | 1.48278 | −1.21184 | −2.02926 |
| Bromine | $Br_2$ | | | | 2.4 | 21.9 | 38.9 | 58.3 | 80.8 | 116.5 | 149.1 | −6.76024 | 1.50339 | −0.64097 | −3.62166 |
| Iodine | $I_2$ | | | | | 134.5 | 157.5 | 183.8 | 214.3 | 262.8 | 307.5 | −6.98158 | 2.33987 | −1.48090 | −3.73441 |
| **Anorganic compounds** | | | | | | | | | | | | | | | |
| Hydrogen fluoride | HF | | −75.2 | −48.4 | −35.2 | −15.7 | 0.8 | 19.2 | 39.7 | 71.0 | 98.3 | −9.73172 | 5.07747 | −2.98832 | 5.51671 |
| Hydrogen chloride | HCl | | | | | −106.5 | −96.6 | −85.3 | −72.1 | −51.2 | −32.1 | −6.63222 | 1.06066 | 0.05415 | −4.45907 |
| Hydrogen bromide | HBr | | | | | | −79.4 | −66.8 | −52.4 | −29.6 | −8.7 | −5.92115 | 0.77533 | −1.67956 | 1.00212 |
| Hydrogen iodide | HI | | | | | | −50.5 | −35.7 | −18.6 | 8.8 | 34.0 | −5.92123 | 0.95693 | −1.04474 | −1.03336 |
| Hydrogen cyanide | HCN | | | | | −7.4 | 8.0 | 25.3 | 45.1 | 75.7 | 103.0 | −9.77338 | 5.29679 | −4.36059 | 1.58018 |
| Water | $H_2O$ | | 7.0 | 32.9 | 45.8 | 65.0 | 81.3 | 99.6 | 120.2 | 151.8 | 179.9 | −7.86975 | 1.90561 | −2.30891 | −2.06472 |
| Hydrogen sulfide | $H_2S$ | | | | | −84.4 | −73.3 | −60.6 | −45.9 | −22.5 | −1.1 | −6.50342 | 1.52011 | −1.36969 | −1.96704 |
| Ammonia | $NH_3$ | | | | −71.2 | −58.0 | −46.5 | −33.6 | −18.8 | 4.1 | 24.9 | −7.30274 | 1.64638 | −2.01606 | −1.96884 |
| Nitric oxide | NO | | | | | | −157.6 | −151.9 | −145.4 | −135.3 | −126.2 | −8.38772 | 0.85755 | −3.11447 | −8.98765 |
| Nitrogen dioxide | $NO_2$ | | | | | −6.2 | 6.8 | 20.9 | 36.4 | 59.3 | 78.7 | −11.33898 | 2.37620 | 0.67820 | −2.53997 |
| Nitrous oxide | $N_2O$ | | | | | | | −88.7 | −76.2 | −56.4 | −38.2 | −6.79599 | 1.59751 | −1.85163 | −2.29494 |
| Dinitrogentetroxide | $N_2O_4$ | | | | | −6.1 | 6.8 | 21.0 | 36.6 | 59.6 | 79.1 | −11.71738 | 3.10196 | 0.59704 | −5.33648 |
| Cyanogen | $C_2N_2$ | | | | | | | −21.4 | −5.1 | 20.7 | 44.3 | −7.51492 | 1.94916 | −2.36750 | −4.23472 |
| Phosphorus trichloride | $PCl_3$ | −35.6 | −25.9 | 0.7 | 14.4 | 35.2 | 53.5 | 74.6 | 99.2 | 138.4 | 174.6 | −8.83133 | 5.61883 | −4.80318 | −1.25347 |
| Cyanogen chloride | ClCN | | | | | | −3.9 | 12.5 | 30.9 | 59.3 | 84.9 | −7.49333 | 1.78753 | −4.04253 | 8.50574 |
| Silane | $SiH_4$ | −167.8 | −163.1 | −150.2 | −143.4 | −132.8 | −123.3 | −112.3 | −99.2 | −78.2 | −58.9 | −7.30552 | 2.71060 | −0.09783 | −4.71464 |
| Tetrachlorosilane | $SiCl_4$ | −47.9 | −38.7 | −13.3 | −0.3 | 19.5 | 36.8 | 56.8 | 79.9 | 116.8 | 151.0 | −6.60174 | 0.34409 | −1.09066 | −3.15050 |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Carbon monoxide | CO | | | | | −202.1 | −197.2 | −191.6 | −185.0 | −174.3 | −164.2 | −6.19574 | 1.32502 | −0.95226 | −1.98513 |
| Carbon dioxide | $CO_2$ | | | | | | | | | | −40.1 | −7.02916 | 1.53937 | −2.28330 | −2.34853 |
| Carbon suboxide | $C_3O_2$ | −82.8 | −74.8 | −53.1 | −41.9 | −25.1 | −10.5 | 6.0 | 24.9 | 53.8 | 78.8 | −13.34201 | 11.51312 | −6.91741 | −0.29406 |
| Carbonyl sulfide | COS | −123.0 | −116.6 | −99.1 | −90.1 | −76.4 | −64.3 | −50.5 | −34.3 | −8.6 | 15.3 | −6.51272 | 1.55373 | −1.33074 | −2.08761 |
| Phosgene | $CCl_2O$ | −80.1 | −72.4 | −51.3 | −40.4 | −23.9 | −9.3 | 7.4 | 26.7 | 57.5 | 85.7 | −6.82435 | 0.89402 | −0.50281 | −4.67598 |
| Carbon disulfide | $CS_2$ | −57.9 | −48.8 | −23.8 | −10.9 | 8.7 | 26.0 | 45.8 | 68.8 | 105.2 | 138.5 | −6.58802 | 1.03676 | 0.15875 | −3.44094 |
| Sulfur dioxide | $SO_2$ | | | −61.9 | −52.1 | −37.5 | −24.8 | −10.3 | 6.3 | 32.5 | 56.3 | −7.27858 | 1.72871 | −2.37473 | −2.70464 |
| Sulfur trioxide | $SO_3$ | | | | | 19.6 | 31.1 | 44.2 | 59.5 | 84.1 | 107.3 | −8.74717 | 6.32513 | −13.93665 | −9.67972 |
| Sulfuryl chloride | $Cl_2SO_2$ | −36.5 | −27.0 | −1.3 | 11.9 | 31.7 | 49.1 | 69.0 | 92.1 | 129.2 | 163.9 | −6.32835 | 0.89929 | −2.88437 | −1.24330 |
| Sulfur hexafluoride | $SF_6$ | | | | | | | | | −29.8 | −8.0 | −7.08034 | 1.65103 | −1.96365 | −0.25060 |
| **Organic compounds containing sulfur** | | | | | | | | | | | | | | | |
| Methyl mercaptan | $CH_4S$ | −81.6 | −73.8 | −52.6 | −41.8 | −25.3 | −10.9 | 5.7 | 24.9 | 55.7 | 84.3 | −8.04229 | 4.64898 | −4.38751 | −1.03684 |
| Ethyl mercaptan | $C_2H_6S$ | −62.2 | −53.6 | −30.1 | −18.0 | 0.3 | 16.3 | 34.7 | 55.9 | 89.7 | 120.8 | −6.85400 | 1.41434 | −1.74027 | −2.40242 |
| Dimethyl sulfide | $C_2H_6S$ | −59.7 | −51.2 | −27.9 | −15.9 | 2.4 | 18.5 | 37.0 | 58.5 | 92.9 | 124.6 | −7.20168 | 1.99080 | −1.67979 | −3.99499 |
| Diethyl sulfide | $C_4H_{10}S$ | −23.6 | −13.1 | 15.4 | 29.8 | 51.5 | 70.3 | 91.7 | 116.3 | 155.0 | 190.5 | −6.90446 | 0.48320 | −1.77018 | −0.12336 |
| Thiophene | $C_4H_4S$ | −26.0 | −16.3 | 10.2 | 23.8 | 44.6 | 62.8 | 83.8 | 108.1 | 147.0 | 182.8 | −7.01021 | 1.63774 | −1.66720 | −4.21813 |
| **Halogenated hydrocarbons** | | | | | | | | | | | | | | | |
| Fluoromethane (R41) | $CH_3F$ | −140.5 | −135.0 | −120.0 | −112.2 | −100.5 | −90.3 | −78.6 | −65.1 | −43.7 | −24.0 | −7.21927 | 1.95643 | −1.73271 | −2.07627 |
| Difluoromethane (R32) | $CH_2F_2$ | −119.6 | −113.5 | −96.9 | −88.5 | −75.7 | −64.6 | −51.9 | −37.3 | −14.3 | 6.6 | −7.47027 | 1.75595 | −2.01429 | −2.62147 |
| Trifluoromethane (R23) | $CHF_3$ | −141.6 | −136.3 | −121.8 | −114.4 | −103.2 | −93.4 | −82.3 | −69.4 | −49.1 | −30.3 | −7.38216 | 1.96234 | −2.68392 | −1.43178 |
| Tetrafluoromethane (R14) | $CF_4$ | −175.8 | −171.6 | −160.3 | −154.4 | −145.4 | −137.4 | −128.3 | −117.6 | −100.4 | −84.6 | −6.92188 | 1.54525 | −1.41276 | −2.87791 |
| Methyl chloride | $CH_3Cl$ | | −96.2 | −77.1 | −67.3 | −52.5 | −39.4 | −24.5 | −7.1 | 20.4 | 45.7 | −6.71862 | 1.27727 | −0.96338 | −3.14698 |
| Methylene chloride | $CH_2Cl_2$ | −56.3 | −47.8 | −24.5 | −12.6 | 5.5 | 21.3 | 39.4 | 60.5 | 94.2 | 125.5 | −7.57368 | 3.17104 | −3.53296 | −2.27696 |
| Chloroform | $CHCl_3$ | −41.8 | −32.9 | −8.2 | 4.5 | 23.9 | 41.0 | 60.7 | 83.6 | 120.0 | 153.4 | −7.32485 | 1.69599 | −0.93627 | −5.89590 |
| Carbon tetrachloride | $CCl_4$ | | | 2.1 | 15.8 | 36.7 | 55.1 | 76.3 | 101.0 | 140.5 | 177.1 | −7.11728 | 1.96174 | −2.05900 | −3.26771 |
| Bromomethane | $CH_3Br$ | −84.4 | −76.6 | −55.3 | −44.4 | −27.8 | −13.3 | 3.3 | 22.4 | 52.7 | 80.2 | −7.65380 | 2.84555 | −1.71564 | −2.54232 |
| Dibromomethane | $CH_2Br_2$ | −16.0 | −6.0 | 21.3 | 35.4 | 56.6 | 75.2 | 96.5 | 121.2 | 160.3 | 196.1 | −7.25658 | 1.92921 | −1.61527 | −4.04404 |
| Tribromomethane | $CHBr_3$ | 18.8 | 30.4 | 62.0 | 78.2 | 102.7 | 124.1 | 148.7 | 177.2 | 223.0 | 265.7 | −7.16326 | 2.92794 | −3.91279 | −1.16341 |
| Tetrabromomethane | $CBr_4$ | | | 95.2 | 111.8 | 137.8 | 161.3 | 188.8 | 220.6 | 269.5 | 310.6 | −13.48480 | 9.03531 | 1.84773 | −22.26830 |
| Chlorodifluoromethane (R22) | $CHClF_2$ | −113.5 | −107.0 | −89.5 | −80.4 | −66.8 | −54.8 | −41.1 | −25.2 | 0.1 | 23.4 | −7.09210 | 1.61905 | −2.01221 | −2.73123 |
| Dichlorofluoromethane (R21) | $CHCl_2F$ | −78.7 | −70.9 | −49.8 | −39.0 | −22.5 | −8.1 | 8.5 | 27.7 | 58.3 | 86.7 | −6.95944 | 1.53177 | −1.97969 | −3.25683 |
| Chlorotrifluoromethane (R13) | $CClF_3$ | −144.2 | −138.7 | −123.7 | −115.9 | −104.1 | −93.7 | −81.7 | −67.7 | −45.2 | −24.4 | −6.82801 | 1.52677 | −1.75147 | −2.23841 |
| Dichlorodifluoromethane (R12) | $CCl_2F_2$ | −108.7 | −101.8 | −82.9 | −73.1 | −58.3 | −45.2 | −30.1 | −12.5 | 15.7 | 41.7 | −6.92085 | 1.62615 | −1.73939 | −2.58282 |
| Trichlorofluoromethane (R11) | $CCl_3F$ | −71.6 | −63.3 | −40.4 | −28.6 | −10.7 | 5.1 | 23.3 | 44.4 | 78.2 | 109.4 | −6.91946 | 1.52457 | −1.66128 | −2.85320 |
| Ethyl fluoride (R161) | $C_2H_5F$ | −113.2 | −106.5 | −88.2 | −78.8 | −64.6 | −52.1 | −38.0 | −21.6 | 4.4 | 28.1 | −7.07032 | 1.42577 | −1.49199 | −1.92623 |
| Ethyl chloride | $C_2H_5Cl$ | −78.2 | −70.2 | −48.3 | −37.1 | −20.1 | −5.2 | 11.9 | 31.7 | 63.4 | 92.7 | −7.36967 | 2.69543 | −3.02790 | −1.39375 |
| Ethyl bromide | $C_2H_5Br$ | −62.1 | −53.0 | −28.2 | −15.7 | 3.1 | 19.5 | 38.1 | 59.5 | 93.7 | 125.1 | −9.71666 | 7.74488 | −7.76676 | 3.99427 |

D3.1. Table 3. (continued)

| Substance | Formula | Vapor pressure in mbar | | | | | | | | | | Equation (7) | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 5 | 10 | 50 | 100 | 250 | 500 | 1,000 | 2,000 | 5,000 | 10,000 | *A* | *B* | *C* | *D* |
| 1,1-Dichloroethane | $C_2H_4C_2H_4Cl_2$ | −45.7 | −36.5 | −11.5 | 1.3 | 20.6 | 37.4 | 56.7 | 78.9 | 114.0 | 146.3 | −6.63204 | 0.36053 | −1.04822 | −2.87286 |
| 1,2-Dichloroethane | $C_2H_4Cl_2$ | −26.2 | −16.4 | 10.2 | 23.8 | 44.4 | 62.5 | 83.2 | 107.2 | 145.1 | 179.8 | −8.26850 | 3.49184 | −3.19752 | −2.97053 |
| 1,2-Dibromoethane | $C_2H_4Br_2$ | | 17.5 | 47.9 | 63.4 | 86.8 | 107.4 | 131.0 | 158.4 | 202.3 | 243.1 | −7.96068 | 4.07852 | −4.74206 | −0.88410 |
| 1,1,1-Trifluoroethane (R143a) | $C_2H_3F_3$ | | | −95.2 | −86.4 | −72.9 | −61.1 | −47.5 | −31.8 | −6.7 | 16.3 | −7.35995 | 1.71203 | −2.01879 | −2.98413 |
| 1,1,1-Trichloroethane | $C_2H_3Cl_3$ | | −25.9 | 0.4 | 14.0 | 34.6 | 52.8 | 73.7 | 98.0 | 136.9 | 172.8 | −7.21356 | 1.90482 | −2.08892 | −3.31006 |
| 1,1,2,2-Tetrachloroethane | $C_2H_2Cl_4$ | 18.0 | 29.5 | 60.9 | 76.9 | 100.9 | 121.7 | 145.4 | 172.7 | 215.9 | 256.0 | −5.60385 | −1.82148 | −0.70234 | −1.88475 |
| Pentachloroethane | $C_2HCl_5$ | 27.3 | 39.2 | 71.5 | 88.1 | 113.1 | 134.9 | 159.9 | 188.7 | 234.6 | 276.7 | −7.59524 | 1.63691 | −2.82337 | −2.34305 |
| Hexachloroethane | $C_2Cl_6$ | | | | | | | | 215.1 | 265.9 | 313.7 | −6.84574 | 1.14406 | −2.27578 | −7.15228 |
| 1,1,2,2-Tetrachlorodifluoroethane | $C_2Cl_4F_2$ | | | | 31.2 | 52.5 | 71.1 | 92.6 | 117.5 | 157.4 | 194.5 | −7.71309 | 2.64672 | −3.98878 | −1.66517 |
| 1,1,2-Trichlorotrifluoroethan | $C_2Cl_3F_3$ | | | −20.7 | −8.1 | 11.0 | 27.8 | 47.2 | 69.8 | 105.9 | 139.3 | −7.24399 | 1.63003 | −2.12928 | −3.49922 |
| 1,2-Dichlorotetrafluoroethane | $C_2Cl_2F_4$ | −84.9 | −77.0 | −55.6 | −44.7 | −28.1 | −13.5 | 3.3 | 22.8 | 54.1 | 83.3 | −7.64719 | 2.95529 | −4.23671 | 0.15959 |
| 1-Chloropropane | $C_3H_7Cl$ | −53.5 | −44.7 | −20.6 | −8.2 | 10.7 | 27.2 | 46.1 | 68.2 | 103.3 | 135.7 | −7.23105 | 1.89946 | −2.29641 | −2.86891 |
| 1-Chlorobutane | $C_4H_9Cl$ | −30.6 | −21.1 | 4.9 | 18.4 | 39.0 | 57.2 | 78.3 | 102.8 | 142.2 | 178.8 | −6.77199 | 0.79529 | −1.25773 | −5.53709 |
| 1-Chloropentane | $C_5H_{11}Cl$ | −11.5 | −1.0 | 27.7 | 42.5 | 65.1 | 85.0 | 108.0 | 134.8 | 177.6 | 216.6 | −9.45097 | 5.86945 | −5.57003 | −2.09598 |
| Chlorotrifluoroethene | $C_2ClF_3$ | −117.7 | −108.5 | −85.3 | −74.1 | −57.9 | −44.3 | −29.1 | −11.8 | 15.5 | 40.7 | −8.22217 | 4.87114 | −7.47925 | 13.31070 |
| Vinyl chloride | $C_2H_3Cl$ | −96.2 | −89.0 | −69.2 | −59.0 | −43.5 | −29.9 | −14.1 | 4.3 | 33.8 | 61.3 | −6.32153 | 1.11198 | −1.35813 | −3.25332 |
| 1,1-Dichloroethene | $C_2H_2Cl_2$ | −63.4 | −55.1 | −32.4 | −20.7 | −2.8 | 13.0 | 31.3 | 52.8 | 87.5 | 119.4 | −10.49400 | 9.03819 | −7.79814 | −1.10724 |
| Trichloroethene | $C_2HCl_3$ | −26.8 | −16.6 | 11.2 | 25.3 | 46.4 | 64.8 | 85.7 | 109.9 | 148.4 | 184.2 | −6.86463 | 1.75400 | −3.57287 | 0.95588 |
| Tetrachloroethene | $C_2Cl_4$ | −2.1 | 8.9 | 39.0 | 54.3 | 77.4 | 97.6 | 120.6 | 147.1 | 189.5 | 228.8 | −6.50488 | 0.75823 | −2.53992 | −0.58809 |
| Fluorobenzene | $C_6H_5F$ | −26.8 | −16.8 | 10.5 | 24.4 | 45.4 | 63.8 | 84.8 | 109.1 | 147.8 | 183.5 | −7.42663 | 2.30457 | −3.23481 | −1.05236 |
| Chlorobenzene | $C_6H_5Cl$ | 5.6 | 16.8 | 47.5 | 63.2 | 86.9 | 107.7 | 131.4 | 159.0 | 202.8 | 243.2 | −7.41321 | 2.18452 | −2.95675 | −1.66197 |
| Bromobenzene | $C_6H_5Br$ | 22.9 | 34.6 | 66.7 | 83.2 | 108.2 | 130.2 | 155.5 | 184.9 | 232.0 | 275.6 | −8.10313 | 3.78791 | −4.14347 | −2.11742 |
| Iodobenzene | $C_6H_5I$ | 45.4 | 58.1 | 92.8 | 110.5 | 137.4 | 160.8 | 187.8 | 219.0 | 268.9 | 315.1 | −7.47909 | 2.53825 | −3.54320 | −1.50458 |
| *m*-Chlorotoluene | $C_7H_7Cl$ | 24.5 | 37.3 | 71.6 | 88.8 | 114.6 | 137.0 | 162.3 | 191.3 | 237.3 | 279.7 | −7.90360 | 2.90903 | −4.76707 | 3.62554 |
| Benzyl chloride | $C_7H_7Cl$ | 42.9 | 55.4 | 89.2 | 106.2 | 131.8 | 153.9 | 179.0 | 207.9 | 253.8 | 296.4 | −6.24204 | −0.59859 | −2.50951 | 0.21300 |
| ***n*-Alkanes** | | | | | | | | | | | | | | | |
| Methane | $CH_4$ | | | | | −176.1 | −169.4 | −161.6 | −152.5 | −137.8 | −124.0 | −6.02388 | 1.26813 | −0.56948 | −1.37648 |
| Ethane | $C_2H_6$ | −150.6 | −145.2 | −130.4 | −122.7 | −111.0 | −100.7 | −88.8 | −75.0 | −52.7 | −32.1 | −6.46252 | 1.35760 | −1.04922 | −2.03789 |
| Propane | $C_3H_8$ | −118.1 | −111.5 | −93.3 | −83.9 | −69.6 | −57.0 | −42.4 | −25.5 | 1.7 | 26.9 | −6.71480 | 1.38388 | −1.30695 | −2.56827 |
| *n*-Butane | $C_4H_{10}$ | −89.0 | −81.3 | −60.0 | −49.1 | −32.4 | −17.7 | −0.8 | 18.8 | 50.3 | 79.5 | −7.08562 | 1.79335 | −2.00003 | −2.31975 |
| *n*-Pentane | $C_5H_{12}$ | −62.8 | −54.1 | −30.4 | −18.1 | 0.5 | 16.9 | 35.7 | 57.6 | 92.6 | 124.9 | −7.36401 | 1.94358 | −2.47191 | −2.34757 |
| *n*-Hexane | $C_6H_{14}$ | −38.9 | −29.5 | −3.6 | 9.8 | 30.0 | 47.8 | 68.3 | 92.1 | 130.1 | 165.1 | −7.61075 | 2.00527 | −2.74158 | −2.82824 |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *n*-Heptane | $C_7H_{16}$ | −16.7 | −6.6 | 21.1 | 35.4 | 57.0 | 76.1 | 98.0 | 123.4 | 163.9 | 201.1 | −7.75469 | 1.84795 | −2.80333 | −3.62418 |
| *n*-Octane | $C_8H_{18}$ | 3.9 | 14.6 | 43.9 | 59.0 | 81.9 | 102.0 | 125.2 | 152.0 | 194.8 | 234.1 | −8.01133 | 1.98859 | −3.26507 | −3.99439 |
| *n*-Nonane | $C_9H_{20}$ | 22.7 | 34.0 | 64.9 | 80.7 | 104.8 | 126.0 | 150.3 | 178.5 | 223.3 | 264.4 | −8.45145 | 2.57850 | −4.17533 | −3.66755 |
| *n*-Decane | $C_{10}H_{22}$ | 40.4 | 52.2 | 84.5 | 101.1 | 126.3 | 148.3 | 173.6 | 202.9 | 249.5 | 292.0 | −8.62717 | 2.55890 | −4.50221 | −3.63420 |
| *n*-Undecane | $C_{11}H_{24}$ | 57.3 | 69.6 | 103.1 | 120.3 | 146.3 | 169.2 | 195.3 | 225.7 | 273.8 | 317.7 | −8.73044 | 2.35716 | −4.52576 | −4.46648 |
| *n*-Dodecane | $C_{12}H_{26}$ | 73.2 | 85.9 | 120.4 | 138.2 | 165.1 | 188.7 | 215.7 | 247.1 | 296.6 | 341.4 | −8.97902 | 2.40530 | −4.55315 | −5.99492 |
| *n*-Tridecane | $C_{13}H_{28}$ | 88.4 | 101.4 | 136.9 | 155.2 | 182.9 | 207.1 | 234.9 | 266.9 | 317.3 | 363.0 | −8.71245 | 1.11086 | −3.15308 | −8.81599 |
| *n*-Tetradecane | $C_{14}H_{30}$ | 102.1 | 115.6 | 152.4 | 171.2 | 199.6 | 224.5 | 252.9 | 285.8 | 338.0 | 385.4 | −8.99672 | 1.98553 | −5.38986 | −4.09226 |
| *n*-Pentadecane | $C_{15}H_{32}$ | 115.8 | 129.5 | 167.1 | 186.3 | 215.4 | 240.9 | 270.0 | 303.5 | 356.4 | 404.4 | −8.86498 | 0.89612 | −3.70098 | −8.72916 |
| *n*-Hexadecane | $C_{16}H_{34}$ | 128.5 | 142.6 | 181.0 | 200.7 | 230.5 | 256.5 | 286.1 | 320.4 | 374.3 | 423.4 | −8.96067 | 0.85195 | −4.04080 | −8.42218 |
| *n*-Heptadecane | $C_{17}H_{36}$ | 141.2 | 155.7 | 195.1 | 215.2 | 245.4 | 271.7 | 301.8 | 336.4 | 390.9 | 440.2 | −9.43782 | 1.65057 | −5.70751 | −4.71679 |
| *n*-Octadecane | $C_{18}H_{38}$ | 152.6 | 167.3 | 207.3 | 227.7 | 258.4 | 285.1 | 315.6 | 350.8 | 406.1 | 455.6 | −9.87775 | 2.42883 | −7.03772 | −3.36978 |
| *n*-Nonadecane | $C_{19}H_{40}$ | 163.9 | 178.8 | 219.3 | 240.0 | 271.2 | 298.5 | 329.5 | 365.1 | 420.8 | 470.3 | −9.91003 | 1.64273 | −5.20678 | −10.43208 |
| *n*-Eicosane | $C_{20}H_{42}$ | 174.7 | 189.8 | 231.1 | 252.2 | 284.0 | 311.7 | 343.1 | 379.0 | 435.2 | 486.5 | −8.99815 | −1.30230 | −1.45511 | −16.74038 |
| **Isoalkanes** | | | | | | | | | | | | | | | |
| Isobutane | $C_4H_{10}$ | −97.2 | −89.8 | −69.4 | −58.8 | −42.7 | −28.5 | −12.1 | 7.0 | 37.7 | 66.2 | −6.90675 | 1.57740 | −1.80160 | −2.42893 |
| 2-Methyl butane | $C_5H_{12}$ | −69.3 | −60.9 | −37.6 | −25.6 | −7.3 | 8.9 | 27.5 | 49.1 | 83.7 | 115.8 | −7.18224 | 1.72845 | −2.05353 | −2.71274 |
| 2,2-Dimethyl propane | $C_5H_{12}$ | | | | | | −8.6 | 9.1 | 29.9 | 63.3 | 94.4 | −6.98355 | 1.67850 | −2.08470 | −2.42800 |
| 2-Methyl pentane | $C_6H_{14}$ | −45.6 | −36.3 | −10.9 | 2.2 | 22.1 | 39.6 | 59.8 | 83.3 | 120.8 | 155.5 | −7.49311 | 1.93828 | −2.57247 | −2.85203 |
| 3-Methyl pentane | $C_6H_{14}$ | −43.8 | −34.4 | −8.7 | 4.6 | 24.7 | 42.4 | 62.8 | 86.6 | 124.7 | 160.0 | −7.76049 | 2.81104 | −3.61863 | −1.53175 |
| 2,2-Dimethyl butane | $C_6H_{14}$ | −54.7 | −45.7 | −20.7 | −7.8 | 11.9 | 29.3 | 49.3 | 72.7 | 110.0 | 144.4 | −6.84403 | 0.74239 | −0.92872 | −4.01577 |
| 2,3-Dimethyl butane | $C_6H_{14}$ | −48.7 | −39.3 | −13.7 | −0.5 | 19.6 | 37.2 | 57.5 | 81.1 | 118.8 | 153.8 | −7.23412 | 1.74312 | −2.49507 | −1.81829 |
| **Olefins** | | | | | | | | | | | | | | | |
| Ethylene | $C_2H_4$ | −160.5 | −155.5 | −142.0 | −135.0 | −124.3 | −114.9 | −104.0 | −91.3 | −70.9 | −51.8 | −6.41327 | 1.45469 | −1.24183 | −1.99446 |
| Propylene | $C_3H_6$ | −121.5 | −115.1 | −97.4 | −88.3 | −74.4 | −62.1 | −48.0 | −31.5 | −5.2 | 19.2 | −6.66599 | 1.43430 | −1.39324 | −2.46883 |
| 1-Butene | $C_4H_8$ | −92.5 | −84.9 | −64.3 | −53.7 | −37.4 | −23.1 | −6.7 | 12.6 | 43.3 | 71.8 | −7.07897 | 1.87819 | −2.02256 | −2.64845 |
| 1-Pentene | $C_5H_{10}$ | −67.1 | −58.7 | −35.4 | −23.4 | −5.1 | 11.0 | 29.6 | 51.2 | 85.6 | 117.4 | −7.23957 | 1.68881 | −1.87158 | −3.19856 |
| 1-Hexene | $C_6H_{12}$ | −42.7 | −33.4 | −8.0 | 5.2 | 25.2 | 42.8 | 63.1 | 86.7 | 124.4 | 159.2 | −7.47396 | 1.85450 | −2.38903 | −3.50639 |
| 1-Heptene | $C_7H_{14}$ | −20.6 | −10.6 | 16.9 | 31.0 | 52.5 | 71.4 | 93.2 | 118.7 | 159.2 | 196.4 | −8.62839 | 3.98397 | −4.58652 | −2.45443 |
| 1-Octene | $C_8H_{16}$ | 0.0 | 10.6 | 39.8 | 54.8 | 77.7 | 97.8 | 120.8 | 147.5 | 189.7 | 228.1 | −7.93750 | 1.47392 | −1.85509 | −5.72867 |
| Propadiene | $C_3H_4$ | −109.8 | −103.4 | −85.8 | −76.6 | −62.4 | −49.6 | −34.7 | −17.1 | 11.8 | 38.9 | −8.00232 | 4.45942 | −2.87994 | −5.85178 |
| 1,2-Butadiene | $C_4H_6$ | −80.9 | −72.7 | −50.4 | −38.9 | −21.7 | −6.7 | 10.5 | 30.4 | 62.1 | 91.5 | −6.07102 | 0.12159 | −1.55692 | −0.53215 |
| 1,3-Butadiene | $C_4H_6$ | −90.8 | −83.3 | −62.6 | −52.0 | −35.7 | −21.4 | −4.8 | 14.4 | 45.1 | 73.5 | −6.79824 | 1.08553 | −0.96279 | −3.84778 |
| 1,2-Pentadiene | $C_5H_8$ | −55.0 | −46.2 | −22.1 | −9.7 | 9.0 | 25.5 | 44.4 | 66.6 | 102.3 | 136.1 | −5.94252 | 0.26690 | −2.35857 | −1.73048 |
| *trans*-1,3-Pentadiene | $C_5H_8$ | −57.9 | −49.1 | −25.0 | −12.6 | 6.2 | 22.6 | 41.6 | 63.8 | 99.7 | 133.9 | −5.50529 | −0.22313 | −2.15448 | −1.34395 |
| 1,4-Pentadiene | $C_5H_8$ | −69.3 | −60.9 | −38.0 | −26.2 | −8.3 | 7.4 | 25.6 | 46.9 | 81.5 | 114.7 | −5.36609 | −0.09618 | −2.39750 | −1.13323 |
| 2,3-Pentadiene | $C_5H_8$ | −51.8 | −43.0 | −18.7 | −6.3 | 12.5 | 29.0 | 47.9 | 69.9 | 105.2 | 138.2 | −6.57492 | 0.82240 | −2.46643 | −2.03177 |

D3.1. Table 3. (continued)

| Substance | Formula | Vapor pressure in mbar | | | | | | | | | | Equation (7) | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 5 | 10 | 50 | 100 | 250 | 500 | 1,000 | 2,000 | 5,000 | 10,000 | *A* | *B* | *C* | *D* |
| **Acetylene and derivatives** | | | | | | | | | | | | | | | |
| Acetylene | $C_2H_2$ | | | | | | | | −72.1 | −51.7 | −32.9 | −6.99241 | 1.57338 | −1.33202 | −5.21884 |
| Propyne | $C_3H_4$ | −100.9 | −93.9 | −75.0 | −65.3 | −50.7 | −38.0 | −23.4 | −6.6 | 20.2 | 44.8 | −7.11026 | 1.86493 | −2.56109 | −1.65671 |
| 2-Butyne | $C_4H_6$ | | | | −23.9 | −6.3 | 9.1 | 26.6 | 46.9 | 79.1 | 108.6 | −6.85375 | 0.83418 | −1.42544 | −2.91847 |
| 1-Butyne | $C_4H_6$ | −79.1 | −71.3 | −50.2 | −39.4 | −23.0 | −8.7 | 7.8 | 26.8 | 57.1 | 85.0 | −7.17126 | 1.56844 | −2.22263 | −2.83839 |
| **Naphthenes** | | | | | | | | | | | | | | | |
| Cyclopropane | $C_3H_6$ | −111.2 | −104.3 | −85.4 | −75.7 | −61.0 | −48.1 | −33.1 | −15.7 | 12.6 | 39.0 | −8.18446 | 5.40338 | −5.26106 | 0.29975 |
| Cyclobutane | $C_4H_8$ | −80.0 | −71.9 | −49.6 | −38.1 | −20.7 | −5.4 | 12.2 | 32.6 | 65.0 | 94.8 | −7.11287 | 1.86338 | −1.59855 | −2.35844 |
| Cyclopentane | $C_5H_{10}$ | −53.7 | −44.7 | −19.9 | −7.1 | 12.3 | 29.3 | 48.8 | 71.5 | 107.8 | 141.3 | −7.00184 | 1.67430 | −1.95254 | −2.43833 |
| Methyl cyclopentane | $C_6H_{12}$ | −37.7 | −28.1 | −1.8 | 11.8 | 32.4 | 50.5 | 71.4 | 95.7 | 134.5 | 170.5 | −7.22687 | 1.83847 | −2.26044 | −2.89788 |
| Ethyl cyclopentane | $C_7H_{14}$ | −15.1 | −4.7 | 23.7 | 38.4 | 60.7 | 80.3 | 102.9 | 129.2 | 171.2 | 209.9 | −7.33383 | 1.58750 | −2.00285 | −3.84956 |
| Propyl cyclopentane | $C_8H_{16}$ | 5.5 | 16.5 | 46.6 | 62.1 | 85.8 | 106.6 | 130.5 | 158.3 | 202.5 | 243.0 | −7.56400 | 1.41441 | −1.85483 | −4.86488 |
| Butyl cyclopentane | $C_9H_{18}$ | 24.6 | 36.3 | 68.2 | 84.5 | 109.2 | 130.9 | 155.9 | 185.0 | 231.7 | 274.9 | −8.82045 | 4.56618 | −6.39502 | 0.04910 |
| Pentyl cyclopentane | $C_{10}H_{20}$ | 42.1 | 54.5 | 87.9 | 105.0 | 130.9 | 153.6 | 179.9 | 210.8 | 261.3 | 309.1 | −8.34838 | 4.60920 | −8.05957 | 2.47945 |
| Hexyl cyclopentane | $C_{11}H_{22}$ | 60.4 | 72.9 | 107.3 | 125.0 | 151.9 | 175.5 | 202.6 | 233.9 | 283.6 | 328.9 | −8.25942 | 1.53284 | −2.79124 | −6.47404 |
| Cyclohexane | $C_6H_{12}$ | | | | 19.2 | 40.3 | 58.9 | 80.3 | 105.2 | 145.1 | 182.0 | −7.00979 | 1.57475 | −1.96820 | −3.26095 |
| Methyl cyclohexane | $C_7H_{14}$ | −17.9 | −7.7 | 20.7 | 35.4 | 57.8 | 77.6 | 100.5 | 127.1 | 169.6 | 208.9 | −6.99290 | 1.02989 | −1.06613 | −4.84894 |
| Ethyl cyclohexane | $C_8H_{16}$ | 4.7 | 15.7 | 46.2 | 61.9 | 85.9 | 107.0 | 131.4 | 159.8 | 205.4 | 247.9 | −6.62098 | 0.32843 | −1.34736 | −4.41951 |
| Propyl cyclohexane | $C_9H_{18}$ | 23.2 | 34.9 | 67.0 | 83.5 | 108.6 | 130.7 | 156.2 | 186.0 | 233.9 | 279.1 | −6.58910 | 0.42832 | −2.35856 | −3.12499 |
| Butyl cyclohexane | $C_{10}H_{20}$ | 41.8 | 54.0 | 87.5 | 104.7 | 130.9 | 153.9 | 180.4 | 211.5 | 261.7 | 309.3 | −6.34269 | −0.12784 | −2.48780 | −3.28017 |
| Pentyl cyclohexane | $C_{11}H_{22}$ | 58.7 | 71.5 | 106.5 | 124.4 | 151.6 | 175.5 | 203.1 | 235.4 | 287.2 | 334.7 | −9.46392 | 5.58832 | −7.94937 | 0.81254 |
| Hexyl cyclohexane | $C_{12}H_{24}$ | 75.6 | 88.9 | 125.0 | 143.4 | 171.3 | 195.9 | 224.1 | 257.0 | 309.7 | 357.8 | −9.74155 | 5.86346 | −8.50766 | 1.30484 |
| Cyclopentene | $C_5H_8$ | −57.1 | −48.1 | −23.7 | −11.1 | 8.0 | 24.7 | 43.9 | 66.2 | 101.7 | 134.5 | −7.05071 | 1.79116 | −2.02594 | −2.17803 |
| Cyclohexene | $C_6H_{10}$ | −29.4 | −19.6 | 7.4 | 21.3 | 42.5 | 61.1 | 82.5 | 107.5 | 147.3 | 184.3 | −7.19079 | 1.97175 | −2.26256 | −3.04106 |
| **Aromatic compounds** | | | | | | | | | | | | | | | |
| Benzene | $C_6H_6$ | | | 6.3 | 20.0 | 40.6 | 58.8 | 79.7 | 103.9 | 142.6 | 178.4 | −7.11451 | 1.83981 | −2.25158 | −3.15179 |
| Toluene | $C_7H_8$ | −9.0 | 1.5 | 30.4 | 45.3 | 67.8 | 87.5 | 110.2 | 136.4 | 178.3 | 216.8 | −7.50051 | 2.08939 | −2.56368 | −2.85042 |
| Ethyl benzene | $C_8H_{10}$ | 9.6 | 20.8 | 51.3 | 67.0 | 90.8 | 111.7 | 135.7 | 163.5 | 207.7 | 248.4 | −7.64476 | 2.01616 | −2.69311 | −3.25571 |
| Propyl benzene | $C_9H_{12}$ | 26.2 | 38.0 | 70.1 | 86.6 | 111.6 | 133.5 | 158.7 | 187.9 | 234.3 | 276.9 | −7.90921 | 2.25623 | −3.18277 | −3.03789 |
| Butyl benzene | $C_{10}H_{14}$ | 44.8 | 57.0 | 90.4 | 107.5 | 133.6 | 156.5 | 182.8 | 213.2 | 261.3 | 305.3 | −7.91469 | 1.51273 | −2.16430 | −5.64758 |
| Pentyl benzene | $C_{11}H_{16}$ | 61.6 | 74.3 | 108.9 | 126.7 | 153.7 | 177.5 | 205.0 | 237.1 | 288.3 | 334.8 | −9.80886 | 6.07290 | −7.50612 | −1.56859 |
| Hexyl benzene | $C_{12}H_{18}$ | 77.4 | 90.5 | 126.4 | 144.8 | 172.7 | 197.3 | 225.6 | 258.5 | 311.0 | 358.4 | −9.64511 | 5.19130 | −6.86455 | −2.47938 |
| *o*-Xylene | $C_8H_{10}$ | 15.6 | 27.0 | 58.1 | 74.1 | 98.4 | 119.6 | 143.9 | 172.1 | 216.8 | 257.9 | −7.60791 | 1.79921 | −2.42215 | −3.36892 |
| *m*-Xylene | $C_8H_{10}$ | 12.1 | 23.3 | 54.0 | 69.8 | 93.7 | 114.6 | 138.6 | 166.4 | 210.5 | 250.9 | −7.63902 | 1.65289 | −2.19801 | −3.94677 |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *p*-Xylene | $C_8H_{10}$ | | 22.2 | 53.0 | 68.8 | 92.8 | 113.8 | 137.9 | 165.8 | 210.0 | 250.6 | −7.67395 | 1.81953 | −2.39673 | −3.44627 |
| 1,2,3-Trimethyl benzene | $C_9H_{12}$ | 38.5 | 50.8 | 84.4 | 101.5 | 127.4 | 149.9 | 175.7 | 205.3 | 252.0 | 294.7 | −7.62987 | 1.23706 | −2.24536 | −2.65979 |
| 1,2,4-Trimethyl benzene | $C_9H_{12}$ | 34.2 | 46.2 | 79.0 | 95.8 | 121.2 | 143.5 | 168.9 | 198.3 | 244.8 | 287.2 | −8.03805 | 2.10078 | −2.99671 | −3.00299 |
| 1,3,5-Trimethyl benzene | $C_9H_{12}$ | 31.3 | 43.2 | 75.7 | 92.3 | 117.3 | 139.2 | 164.2 | 193.0 | 238.4 | 279.7 | −7.82434 | 1.27065 | −2.17890 | −3.60299 |
| 1,2,3,4-Tetramethyl benzene | $C_{10}H_{14}$ | 61.0 | 73.9 | 108.8 | 126.7 | 153.7 | 177.4 | 204.6 | 236.2 | 286.5 | 332.6 | −9.61420 | 5.81425 | −7.22553 | −0.17754 |
| 1,2,3,5-Tetramethyl benzene | $C_{10}H_{14}$ | 56.4 | 69.1 | 103.5 | 121.1 | 147.7 | 170.9 | 197.6 | 228.3 | 277.2 | 321.9 | −8.71211 | 3.45458 | −5.00258 | −1.61174 |
| 1,2,4,5-Tetramethyl benzene | $C_{10}H_{14}$ | | | 102.2 | 119.9 | 146.5 | 169.7 | 196.2 | 226.8 | 275.0 | 319.1 | −7.76585 | 0.96770 | −2.26413 | −3.93132 |
| Pentamethyl benzene | $C_{11}H_{16}$ | 80.3 | 93.9 | 131.0 | 149.8 | 178.2 | 202.9 | 230.9 | 263.1 | 313.7 | 359.8 | −8.00728 | 1.10336 | −2.69076 | −2.48217 |
| Hexamethyl benzene | $C_{12}H_{18}$ | | | | 179.3 | 208.4 | 233.8 | 262.9 | 296.5 | 349.7 | 398.5 | −8.54789 | 2.39022 | −4.64673 | −4.09546 |
| Styrene | $C_8H_8$ | 17.1 | 28.4 | 59.4 | 75.2 | 99.4 | 120.5 | 144.9 | 173.3 | 218.7 | 260.6 | −8.15126 | 3.51813 | −4.34082 | −2.42333 |
| Isopropyl benzene | $C_9H_{12}$ | 21.7 | 33.2 | 64.6 | 80.8 | 105.5 | 127.1 | 151.9 | 180.7 | 226.6 | 268.8 | −7.53496 | 1.50829 | −2.32928 | −4.31012 |
| Biphenyl | $C_{12}H_{10}$ | 97.0 | 111.1 | 149.7 | 169.4 | 199.2 | 225.1 | 254.7 | 288.9 | 342.9 | 392.4 | −7.75945 | 1.70606 | −2.96632 | −3.06189 |
| Diphenyl methane | $C_{13}H_{12}$ | 105.4 | 119.5 | 158.1 | 177.9 | 207.8 | 234.0 | 264.0 | 298.6 | 353.1 | 402.4 | −8.53233 | 2.00873 | −2.93179 | −6.03029 |
| Triphenyl methane | $C_{19}H_{16}$ | 178.3 | 194.6 | 238.8 | 261.3 | 295.3 | 324.9 | 358.8 | 397.9 | 459.9 | 516.6 | −8.84156 | 2.41421 | −5.56532 | −2.75668 |
| Tetraphenyl methane | $C_{25}H_{20}$ | | | 330.3 | 356.3 | 395.6 | 429.8 | 468.9 | 514.0 | 585.3 | 649.7 | −9.59635 | 3.13229 | −6.82319 | −2.76211 |
| Naphthalene | $C_{10}H_8$ | | 80.6 | 117.1 | 135.8 | 164.1 | 188.9 | 217.4 | 250.4 | 303.0 | 351.4 | −7.97682 | 2.86601 | −3.50249 | −2.67778 |
| 1-Methylnaphthalene | $C_{11}H_{10}$ | 86.8 | 100.9 | 139.4 | 159.0 | 188.7 | 214.5 | 243.9 | 277.8 | 331.2 | 380.1 | −6.84372 | −0.39471 | −0.79459 | −3.92723 |
| 2-Methylnaphthalene | $C_{11}H_{10}$ | 85.6 | 99.2 | 136.6 | 155.8 | 185.1 | 211.0 | 241.0 | 276.1 | 332.4 | 383.7 | −10.50759 | 8.20742 | −8.41116 | −1.58015 |
| 1-Ethylnaphthalene | $C_{12}H_{12}$ | 99.8 | 113.9 | 152.3 | 171.9 | 201.6 | 227.7 | 257.6 | 292.3 | 347.6 | 398.3 | −9.12884 | 4.70431 | −6.05976 | −1.87388 |
| 2-Ethylnaphthalene | $C_{12}H_{12}$ | 96.8 | 111.0 | 150.0 | 170.1 | 200.5 | 227.2 | 257.8 | 293.0 | 348.3 | 398.1 | −8.42943 | 2.12066 | −1.95832 | −6.02831 |
| **Alcohols** | | | | | | | | | | | | | | | |
| Methanol | $CH_4O$ | −29.3 | −20.4 | 3.4 | 15.2 | 32.7 | 47.5 | 64.1 | 82.8 | 111.4 | 136.6 | −8.72963 | 1.45860 | −2.78449 | −0.70669 |
| Ethanol | $C_2H_6O$ | −15.7 | −6.7 | 17.2 | 29.0 | 46.5 | 61.4 | 77.9 | 96.6 | 125.2 | 150.7 | −8.33803 | 0.08720 | −3.30575 | −0.26001 |
| 1-Propanol | $C_3H_8O$ | 0.7 | 9.9 | 34.3 | 46.4 | 64.3 | 79.6 | 96.8 | 116.3 | 146.8 | 174.5 | −8.60671 | 2.17353 | −8.04678 | 3.69194 |
| 1-Butanol | $C_4H_{10}O$ | 16.8 | 26.3 | 51.5 | 64.1 | 82.9 | 99.1 | 117.4 | 138.3 | 171.4 | 201.9 | −8.33120 | 2.05530 | −8.17754 | 0.19316 |
| 1-Pentanol | $C_5H_{12}O$ | 30.6 | 40.4 | 66.8 | 80.1 | 100.2 | 117.6 | 137.5 | 160.3 | 196.4 | 229.6 | −8.62225 | 2.10135 | −6.29175 | −6.79293 |
| 1-Hexanol | $C_6H_{14}O$ | 44.9 | 55.2 | 83.0 | 97.0 | 118.1 | 136.4 | 157.3 | 181.5 | 220.1 | 256.1 | −9.17319 | 4.30846 | −10.11890 | −0.93221 |
| 1-Heptanol | $C_7H_{16}O$ | 59.9 | 70.3 | 98.4 | 112.8 | 134.7 | 153.9 | 176.1 | 202.0 | 243.7 | 282.4 | −8.85687 | 3.21033 | −7.48606 | −12.12938 |
| 1-Octanol | $C_8H_{18}O$ | 72.5 | 83.4 | 113.0 | 128.2 | 151.2 | 171.4 | 194.8 | 222.1 | 266.4 | 307.4 | −10.26829 | 6.70186 | −11.65601 | −6.37873 |
| Isopropanol | $C_3H_8O$ | −8.9 | −0.3 | 22.7 | 34.1 | 51.1 | 65.6 | 81.9 | 100.4 | 129.3 | 155.6 | −8.44737 | 1.17402 | −6.97876 | 0.69248 |
| 2-Methyl-1-propanol | $C_4H_{10}O$ | 11.8 | 20.5 | 44.2 | 56.2 | 74.2 | 89.7 | 107.5 | 127.9 | 160.2 | 190.0 | −7.82960 | 0.44510 | −5.32308 | −10.00835 |
| 3-Methyl-1-butanol | $C_5H_{12}O$ | 27.6 | 36.9 | 62.3 | 75.2 | 94.6 | 111.5 | 130.9 | 153.1 | 188.4 | 220.8 | −8.27417 | 1.16334 | −5.04768 | −11.64372 |
| Ethylene glycol | $C_2H_6O_2$ | 75.1 | 86.6 | 117.3 | 132.7 | 155.4 | 174.8 | 196.6 | 221.3 | 259.7 | 294.2 | −7.85575 | 1.06762 | −5.14271 | −1.65660 |
| 1,3-Propylene glycol | $C_3H_8O_2$ | 85.6 | 97.8 | 130.2 | 146.4 | 170.4 | 190.9 | 213.7 | 239.1 | 277.7 | 311.2 | −10.42988 | 2.74631 | −2.20347 | −6.30476 |
| Glycerol | $C_3H_8O_3$ | 147.5 | 160.8 | 196.2 | 213.9 | 239.9 | 262.2 | 287.2 | 315.6 | 359.8 | 400.1 | −6.94758 | −0.33345 | −5.98569 | −1.33011 |
| Cyclohexanol | $C_6H_{12}O$ | 47.1 | 57.3 | 84.8 | 98.8 | 120.2 | 138.9 | 160.4 | 185.6 | 226.3 | 264.7 | −6.96569 | 0.93439 | −5.00403 | −10.29700 |
| Benzyl alcohol | $C_7H_8O$ | 74.9 | 86.7 | 118.5 | 134.6 | 158.8 | 179.9 | 204.0 | 232.0 | 276.9 | 319.2 | −7.38172 | 2.18313 | −6.78536 | −2.57851 |

D3.1. Table 3. (continued)

| Substance | Formula | Vapor pressure in mbar | | | | | | | | | | Equation (7) | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 5 | 10 | 50 | 100 | 250 | 500 | 1,000 | 2,000 | 5,000 | 10,000 | *A* | *B* | *C* | *D* |
| **Phenols** | | | | | | | | | | | | | | | |
| *o*-Cresol | $C_7H_8O$ | 60.1 | 71.8 | 103.6 | 119.9 | 144.4 | 165.8 | 190.3 | 218.6 | 263.2 | 303.8 | −8.83275 | 3.46650 | −4.36291 | −6.10327 |
| *m*-Cresol | $C_7H_8O$ | 70.8 | 82.7 | 114.9 | 131.2 | 155.8 | 177.2 | 201.7 | 229.9 | 274.8 | 316.1 | −8.84466 | 4.00993 | −6.76021 | −3.02124 |
| *p*-Cresol | $C_7H_8O$ | 72.0 | 83.6 | 115.2 | 131.3 | 155.6 | 177.0 | 201.5 | 229.9 | 275.0 | 316.2 | −11.38986 | 9.13086 | −10.26796 | −3.81158 |
| Phenol | $C_6H_6O$ | 55.5 | 67.0 | 98.0 | 113.8 | 137.4 | 158.0 | 181.4 | 208.5 | 251.5 | 290.9 | −10.48951 | 7.87328 | −9.54201 | −0.49292 |
| **Carboxylic acids** | | | | | | | | | | | | | | | |
| Formic acid | $CH_2O_2$ | | | 22.3 | 37.0 | 59.2 | 78.4 | 100.2 | 125.0 | 163.7 | 198.4 | −7.48216 | 0.88805 | −0.32253 | −2.58053 |
| Acetic acid | $C_2H_4O_2$ | | | 41.2 | 55.7 | 77.5 | 96.3 | 117.5 | 141.6 | 179.1 | 212.5 | −9.34304 | 3.77735 | −3.59092 | −1.57006 |
| Propionic acid | $C_3H_6O_2$ | 23.7 | 34.8 | 64.3 | 79.0 | 100.9 | 119.7 | 140.8 | 164.7 | 201.7 | 234.9 | −9.05245 | 2.46694 | −4.73604 | 1.29659 |
| Butyric acid | $C_4H_8O_2$ | 46.8 | 57.6 | 86.8 | 101.4 | 123.2 | 142.0 | 163.2 | 187.4 | 225.0 | 258.8 | −9.92279 | 3.73064 | −6.94231 | −1.65235 |
| Valeric acid | $C_5H_{10}O_2$ | 54.9 | 66.0 | 96.0 | 111.1 | 133.6 | 153.1 | 175.1 | 200.2 | 239.3 | 274.5 | −9.07960 | 1.91018 | −4.75458 | −4.73450 |
| Caproic acid | $C_6H_{12}O_2$ | 82.1 | 93.5 | 123.9 | 139.2 | 162.0 | 181.7 | 204.0 | 229.7 | 270.3 | 307.8 | −9.90505 | 4.66763 | −11.56156 | 2.59120 |
| Acetic anhydride | $C_4H_6O_3$ | 20.7 | 31.5 | 60.7 | 75.5 | 97.8 | 117.1 | 139.1 | 164.3 | 204.0 | 240.2 | −8.15436 | 1.80785 | −3.76039 | −3.04616 |
| Propionic anhydride | $C_6H_{10}O_3$ | 37.5 | 50.2 | 83.5 | 99.8 | 123.8 | 144.0 | 166.5 | 191.9 | 231.3 | 267.1 | −6.66964 | −2.70670 | −1.76623 | 7.54170 |
| Chloroacetic acid | $C_2H_3Cl\,O_2$ | 67.3 | 78.4 | 108.4 | 123.5 | 146.3 | 166.0 | 188.6 | 214.5 | 255.6 | 293.3 | −10.72534 | 7.62232 | −10.44634 | −2.56382 |
| Dichloroacetic acid | $C_2H_2Cl_2O_2$ | 69.5 | 80.7 | 111.0 | 126.5 | 149.8 | 170.2 | 193.5 | 220.3 | 262.7 | 301.1 | −10.38040 | 6.03907 | −7.42780 | −7.72727 |
| Trichloroacetic acid | $C_2HCl_3O_2$ | 70.5 | 82.3 | 114.1 | 130.0 | 153.7 | 174.1 | 197.2 | 223.6 | 265.1 | 302.8 | −8.80390 | 2.91469 | −6.75915 | −0.26065 |
| **Ketones** | | | | | | | | | | | | | | | |
| Ketene | $C_2H_2O$ | −121.4 | −114.9 | −97.4 | −88.5 | −75.0 | −63.3 | −50.0 | −34.6 | −10.1 | 12.6 | −5.93228 | 0.34819 | −1.82981 | −0.11750 |
| Acetone | $C_3H_6O$ | −44.6 | −35.7 | −11.2 | 1.4 | 20.3 | 36.8 | 55.7 | 77.5 | 111.9 | 143.3 | −7.67033 | 1.96469 | −2.44380 | −2.90162 |
| Methyl ethyl ketone | $C_4H_8O$ | −28.9 | −19.2 | 7.4 | 20.9 | 41.2 | 59.0 | 79.2 | 102.5 | 139.4 | 173.2 | −7.89149 | 2.46953 | −3.52510 | −0.92713 |
| Diethyl ketone | $C_5H_{10}O$ | −11.4 | −1.3 | 26.2 | 40.3 | 61.6 | 80.2 | 101.4 | 125.9 | 164.7 | 200.2 | −7.27265 | 0.63120 | −1.64177 | −4.36962 |
| Dipropyl ketone | $C_7H_{14}O$ | 18.2 | 29.3 | 59.9 | 75.5 | 99.2 | 120.0 | 143.7 | 171.1 | 214.5 | 254.0 | −7.98923 | 1.58266 | −2.61251 | −4.38408 |
| Acetophenone | $C_8H_8O$ | 60.3 | 73.0 | 107.7 | 125.4 | 152.1 | 175.4 | 201.9 | 232.4 | 280.4 | 324.2 | −6.96667 | −0.37241 | −0.80507 | −4.88404 |
| Benzophenone | $C_{13}H_{10}O$ | 138.2 | 153.2 | 194.0 | 214.8 | 246.2 | 273.6 | 305.0 | 341.3 | 398.8 | 450.9 | −10.03049 | 5.92909 | −7.69343 | −1.20468 |
| **Ethers** | | | | | | | | | | | | | | | |
| Dimethyl ether | $C_2H_6O$ | −103.8 | −96.7 | −77.5 | −67.6 | −52.8 | −39.9 | −25.1 | −8.0 | 19.3 | 44.5 | −7.33288 | 2.67700 | −3.40250 | −0.11957 |
| Diethyl ether | $C_4H_{10}O$ | −61.3 | −52.8 | −29.7 | −17.8 | 0.2 | 16.0 | 34.1 | 55.1 | 88.7 | 119.7 | −7.55709 | 2.15613 | −3.02766 | −2.37858 |
| Dipropyl ether | $C_6H_{14}O$ | −21.9 | −12.0 | 15.0 | 28.8 | 49.9 | 68.3 | 89.6 | 114.2 | 153.4 | 189.1 | −8.55629 | 3.49469 | −4.22192 | −2.61530 |
| Methyl propyl ether | $C_4H_{10}O$ | −57.9 | −49.4 | −26.1 | −14.1 | 4.1 | 20.1 | 38.5 | 60.1 | 94.8 | 127.1 | −8.76101 | 5.30514 | −6.07025 | −0.78235 |
| Ethyl propyl ether | $C_5H_{12}O$ | −39.8 | −30.9 | −6.3 | 6.4 | 25.9 | 43.2 | 63.4 | 87.1 | 125.2 | 160.0 | −10.68465 | 8.88906 | −8.58949 | −2.06505 |
| Ethylene oxide | $C_2H_4O$ | −76.9 | −69.1 | −47.9 | −37.1 | −20.6 | −6.2 | 10.2 | 29.1 | 58.9 | 86.0 | −6.39656 | −0.13545 | 0.30047 | −4.54866 |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Furane | $C_4H_4O$ | −64.6 | −55.8 | −32.1 | −20.1 | −2.2 | 13.3 | 31.0 | 51.4 | 84.1 | 114.6 | −7.98347 | 4.71720 | −6.64737 | 3.77132 |
| 1,4-Dioxane | $C_4H_8O_2$ | | | 24.8 | 39.3 | 61.0 | 79.7 | 101.0 | 125.4 | 163.9 | 199.3 | −7.40401 | 2.12025 | −3.88819 | 1.69876 |
| **Aldehydes** | | | | | | | | | | | | | | | |
| Formaldehyde | $CH_2O$ | | −90.5 | −71.5 | −61.7 | −47.0 | −34.1 | −19.4 | −2.6 | 23.8 | 47.7 | −7.46907 | 1.28290 | −0.50464 | −4.29089 |
| Acetaldehyde | $C_2H_4O$ | −71.0 | −62.8 | −40.7 | −29.3 | −12.2 | 2.8 | 19.9 | 39.6 | 70.8 | 99.2 | −7.48323 | 1.89754 | −1.87991 | −2.74165 |
| Paraldehyde | $C_6H_{12}O_3$ | | 18.9 | 47.2 | 61.6 | 83.3 | 102.2 | 123.8 | 148.7 | 188.1 | 224.3 | −8.39247 | 2.66850 | −4.68103 | −2.64044 |
| Furfural | $C_5H_4O_2$ | 32.9 | 44.7 | 76.4 | 92.5 | 116.6 | 137.4 | 160.9 | 187.8 | 229.7 | 267.6 | −7.19466 | 0.15098 | −1.29504 | −2.81404 |
| Benzaldehyde | $C_7H_6O$ | 42.3 | 54.5 | 87.6 | 104.6 | 130.2 | 152.7 | 178.3 | 208.0 | 254.8 | 297.6 | −7.62714 | 1.75696 | −2.27084 | −3.91930 |
| Salicylaldehyde | $C_7H_6O_2$ | 55.1 | 68.2 | 103.5 | 121.3 | 147.8 | 170.5 | 195.8 | 224.1 | 267.0 | 304.2 | −10.08822 | 2.82918 | −0.83177 | −3.21642 |
| **Esters** | | | | | | | | | | | | | | | |
| Methyl formate | $C_2H_4O_2$ | −60.4 | −52.1 | −29.6 | −18.1 | −0.8 | 14.2 | 31.4 | 51.2 | 82.5 | 111.3 | −7.09661 | 1.33571 | −2.14672 | −2.79247 |
| Ethyl formate | $C_3H_6O_2$ | −43.7 | −35.0 | −11.4 | 0.7 | 19.0 | 35.1 | 53.6 | 75.0 | 109.1 | 140.5 | −7.17811 | 1.31054 | −2.17904 | −4.85150 |
| Propyl formate | $C_4H_8O_2$ | −25.1 | −15.7 | 10.0 | 23.1 | 43.1 | 60.6 | 80.6 | 103.9 | 141.1 | 175.4 | −7.55263 | 1.95726 | −3.16613 | −3.81792 |
| Methyl acetate | $C_3H_6O_2$ | −42.1 | −33.2 | −9.0 | 3.3 | 21.9 | 38.1 | 56.6 | 78.0 | 112.0 | 143.2 | −8.57584 | 4.22791 | −5.37346 | −0.82045 |
| Ethyl acetate | $C_4H_8O_2$ | −27.4 | −18.0 | 7.4 | 20.4 | 40.0 | 57.1 | 76.7 | 99.4 | 135.4 | 168.4 | −7.89734 | 2.16798 | −3.52390 | −3.10641 |
| Propyl acetate | $C_5H_{10}O_2$ | −9.7 | 0.2 | 27.0 | 40.8 | 61.8 | 80.1 | 101.1 | 125.4 | 164.0 | 199.3 | −7.89781 | 1.68898 | −2.74051 | −5.47967 |
| Methyl propionate | $C_4H_8O_2$ | −25.7 | −16.2 | 9.4 | 22.5 | 42.2 | 59.4 | 79.1 | 102.0 | 138.4 | 172.0 | −8.30872 | 3.53745 | −5.20774 | −1.27089 |
| Ethyl propionate | $C_5H_{10}O_2$ | −11.5 | −1.7 | 25.1 | 38.8 | 59.6 | 77.7 | 98.5 | 122.7 | 161.4 | 197.0 | −8.75519 | 4.14793 | −5.89411 | −1.78473 |
| Propyl propionate | $C_6H_{12}O_2$ | 3.7 | 14.5 | 43.6 | 58.5 | 80.7 | 100.1 | 122.0 | 147.2 | 186.8 | 222.9 | −7.79443 | 0.71065 | −2.20915 | −2.58752 |
| Methyl butyrate | $C_5H_{10}O_2$ | −9.5 | 0.6 | 27.9 | 41.8 | 62.8 | 81.2 | 102.3 | 126.6 | 165.6 | 201.5 | −8.52321 | 3.78350 | −5.74769 | −0.69681 |
| Ethyl butyrate | $C_6H_{12}O_2$ | 0.3 | 11.1 | 40.6 | 55.7 | 78.4 | 98.3 | 120.9 | 147.1 | 188.5 | 226.2 | −8.18197 | 2.21896 | −3.32406 | −2.03342 |
| Methyl benzoate | $C_8H_8O2$ | 60.0 | 72.3 | 105.8 | 123.1 | 149.3 | 172.4 | 198.9 | 229.7 | 278.6 | 323.1 | −9.52872 | 5.22508 | −5.67192 | −4.59960 |
| Ethyl benzoate | $C_9H_{10}O_2$ | 70.8 | 83.0 | 117.0 | 134.6 | 161.5 | 185.3 | 212.8 | 244.5 | 294.5 | 339.0 | −9.49777 | 3.93518 | −3.00984 | −10.93022 |
| Methyl salicylate | $C_8H_8O_3$ | 78.0 | 89.2 | 121.0 | 138.2 | 165.4 | 190.4 | 220.0 | 254.6 | 307.4 | 350.7 | −14.30891 | 11.86128 | −2.67256 | −30.85630 |
| **Amines** | | | | | | | | | | | | | | | |
| Methyl amine | $CH_5N$ | −83.8 | −76.8 | −57.7 | −48.1 | −33.5 | −21.0 | −6.7 | 9.7 | 35.4 | 58.9 | −6.93594 | 0.77016 | −2.12846 | −3.11687 |
| Ethyl amine | $C_2H_7N$ | −69.1 | −61.3 | −40.4 | −29.7 | −13.6 | 0.5 | 16.5 | 34.9 | 64.1 | 90.9 | −7.14146 | 1.24486 | −2.55143 | −3.09059 |
| Propyl amine | $C_3H_9N$ | −48.5 | −39.7 | −16.1 | −4.2 | 13.8 | 29.5 | 47.2 | 67.6 | 99.9 | 129.7 | −6.32807 | −0.41527 | −1.86755 | −1.82733 |
| *n*-butyl amine | $C_6H_{15}N$ | −27.3 | −17.9 | 7.6 | 20.7 | 40.3 | 57.5 | 77.1 | 99.8 | 135.9 | 169.2 | −7.88889 | 2.67770 | −4.27421 | −1.85122 |
| Dimethyl amine | $C_2H_7N$ | −74.4 | −67.1 | −47.3 | −37.2 | −22.0 | −8.7 | 6.6 | 24.4 | 52.9 | 79.4 | −8.48833 | 4.67224 | −6.24955 | −1.96675 |
| Trimethyl amine | $C_3H_9N$ | −84.8 | −77.3 | −56.4 | −45.5 | −28.9 | −14.2 | 2.8 | 22.6 | 54.4 | 83.7 | −7.30365 | 1.94801 | −1.34682 | −5.07582 |
| Diethyl amine | $C_6H_{15}N$ | −46.1 | −36.9 | −12.0 | 0.7 | 19.7 | 36.3 | 55.2 | 77.1 | 111.9 | 144.1 | −7.36200 | 1.77888 | −3.69788 | 0.28823 |
| Triethyl amine | $C_6H_{15}N$ | −24.6 | −14.5 | 13.0 | 27.1 | 48.4 | 67.0 | 88.4 | 113.1 | 152.6 | 189.2 | −7.73549 | 2.33990 | −3.77932 | −0.63259 |
| Piperidine | $C_5H_{11}N$ | | −0.7 | 28.1 | 42.7 | 64.8 | 84.0 | 105.9 | 131.2 | 171.2 | 208.3 | −6.79875 | 1.00957 | −2.60941 | −0.67208 |
| Pyridine | $C_6H_7N$ | −2.9 | 7.6 | 36.3 | 51.0 | 73.2 | 92.6 | 114.8 | 140.4 | 181.1 | 218.6 | −7.07868 | 1.45189 | −2.11714 | −3.20359 |
| Aniline | $C_6H_7N$ | 51.2 | 63.3 | 96.0 | 112.6 | 137.4 | 159.0 | 183.4 | 211.5 | 255.6 | 295.9 | −7.86006 | 1.96206 | −3.65571 | −2.00622 |
| *N*-methyl aniline | $C_7H_9N$ | 57.4 | 69.9 | 104.0 | 121.2 | 147.2 | 169.7 | 195.1 | 224.0 | 269.0 | 309.0 | −8.99983 | 2.75304 | −2.46251 | −3.78980 |

D3.1. Table 3. (continued)

| Substance | Formula | Vapor pressure in mbar | | | | | | | | | | Equation (7) | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 5 | 10 | 50 | 100 | 250 | 500 | 1,000 | 2,000 | 5,000 | 10,000 | *A* | *B* | *C* | *D* |
| *N*,*N*-dimethyl aniline | $C_8H_{11}N$ | 52.0 | 65.0 | 100.0 | 117.7 | 144.2 | 167.1 | 192.9 | 222.4 | 268.6 | 310.8 | −6.91926 | −0.79562 | −1.01346 | −1.30692 |
| *N*,*N*-diethyl aniline | $C_{10}H_{15}N$ | 73.6 | 86.6 | 121.6 | 139.3 | 166.0 | 189.1 | 215.5 | 246.0 | 294.7 | 340.1 | −7.13341 | 0.21353 | −3.88149 | −0.98901 |
| Phenylhydrazine | $C_6H_8N_2$ | 93.8 | 107.0 | 143.4 | 162.1 | 190.4 | 215.2 | 243.4 | 275.7 | 325.9 | 370.0 | −10.65944 | 5.59074 | −3.56952 | −8.23026 |
| Diphenyl amine | $C_{12}H_{11}N$ | 134.0 | 149.3 | 190.7 | 211.7 | 243.3 | 270.7 | 301.8 | 337.3 | 392.8 | 442.8 | −8.75985 | 2.00629 | −3.23950 | −3.32510 |
| **Nitriles** | | | | | | | | | | | | | | | |
| Acetonitrile | $C_2H_3N$ | −31.0 | −20.6 | 7.3 | 21.4 | 42.3 | 60.5 | 81.0 | 104.6 | 141.9 | 175.9 | −9.22263 | 5.68045 | −6.67111 | 4.51306 |
| Propionitrile | $C_3H_5N$ | −17.9 | −7.7 | 20.4 | 34.7 | 56.5 | 75.5 | 97.3 | 122.3 | 161.8 | 197.6 | −7.82826 | 1.87534 | −1.74704 | −3.40003 |
| Butyronitrile | $C_4H_7N$ | −2.0 | 8.6 | 37.6 | 52.4 | 74.8 | 94.4 | 117.0 | 143.0 | 184.4 | 222.0 | −9.07674 | 4.63491 | −4.96526 | −1.94727 |
| Benzonitrile | $C_7H_5N$ | 51.3 | 63.4 | 96.8 | 114.1 | 140.4 | 163.6 | 190.3 | 221.2 | 270.1 | 314.2 | −8.76503 | 3.46762 | −2.58071 | −7.03902 |
| **Amides** | | | | | | | | | | | | | | | |
| Formamide | $CH_3NO$ | 82.2 | 94.8 | 129.0 | 146.2 | 171.9 | 194.0 | 219.1 | 247.6 | 292.1 | 332.3 | −8.05102 | 1.89555 | −3.34638 | −3.18188 |
| **Nitroderivates** | | | | | | | | | | | | | | | |
| Nitromethane | $CH_3NO_2$ | −11.8 | −1.7 | 26.0 | 40.1 | 61.3 | 79.8 | 100.8 | 124.9 | 162.6 | 196.7 | −8.40409 | 2.96310 | −2.55125 | −3.12626 |
| Nitrobenzene | $C_6H_5NO_2$ | 65.8 | 78.5 | 113.5 | 131.4 | 158.7 | 182.6 | 210.2 | 242.1 | 292.6 | 337.8 | −11.42180 | 9.08136 | −8.03968 | −2.40144 |
| *o*-Nitrotoluene | $C_7H_7NO_2$ | 75.0 | 88.0 | 123.6 | 141.8 | 169.4 | 193.5 | 220.9 | 252.4 | 301.5 | 345.5 | −9.20649 | 3.25360 | −2.90528 | −5.87732 |
| *m*-Nitrotoluene | $C_7H_7NO_2$ | 81.8 | 95.3 | 132.1 | 150.9 | 179.3 | 204.0 | 232.1 | 264.4 | 314.8 | 359.8 | −9.97904 | 5.05231 | −4.85807 | −3.04363 |
| *p*-Nitrotoluene | $C_7H_7NO_2$ | 85.1 | 98.9 | 136.2 | 155.3 | 184.1 | 209.3 | 238.1 | 271.5 | 324.6 | 373.0 | −9.14840 | 4.60236 | −6.10485 | −0.71761 |