**Appendix 1.**

Physicochemical properties of octanes.

MW: 114.232

To notate the isomers of octanes the IUPAC Nomenclature was applied. The structures of alkanes are presented in shorthand, e.g. Oct is *n*-octane, 223M5 is 2,2,3-trimethylpentane, 3Et2M5 is 3-ethyl-2-methylpentane, etc.

| PCP \ Octane | Oct | 2M7 | 3M7 | 4M7 | 3Et6 | 25M6 | 24M6 | 23M6 | 34M6 | 3Et2M5 | 22M6 | 33M6 | 3Et3M5 | 234M5 | 224M5 | 223M5 | 233M5 | 2233M4 | Octane \ PCP |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ST | 21.76 | 20.6 | 21.17 | 21.17 | 21.51 | 19.73 | 20.05 | 20.99 | 21.64 | 21.52 | 19.6 | 20.63 | 21.99 | 21.14 | 18.77 | 20.67 | 21.56 | | ST |
| BON | -19 | 13 | 30 | 31 | 49 | 56 | 65 | 71 | 67 | 76 | 67 | 73 | 77 | 97 | 100 | 105 | 100 | | BON |
| RON | -19 | 21.7 | 26.8 | 26.7 | 33.5 | 55.5 | 65.2 | 71.3 | 76.3 | 87.3 | 72.5 | 75.5 | 80.8 | 102.7 | 100 | 109.6 | 106.1 | | RON |
| MON | -19 | 23.8 | 35 | 39 | 52.4 | 55.7 | 69.9 | 78.9 | 81.7 | 88.1 | 77.4 | 83.4 | 88.7 | 95.9 | 100 | 99.9 | 99.4 | | MON |
| S | 111.67 | 109.84 | 111.26 | 109.23 | 109.43 | 105.72 | 106.98 | 108.02 | 106.59 | 106.06 | 103.42 | 104.74 | 101.48 | 102.39 | 104.09 | 101.31 | 102.06 | 93.06 | S |
| $R^2$ | 2.0449 | 1.8913 | 1.7984 | 1.7673 | 1.7673 | 1.6449 | 1.6142 | 1.6464 | 1.523 | 1.5525 | 1.6744 | 1.7377 | 1.5214 | 1.3698 | 1.401 | 1.4306 | 1.4931 | 1.4612 | $R^2$ |
| MR | 39.19 | 39.23 | 39.25 | 39.12 | 38.96 | 39.27 | 38.92 | 38.98 | 38.81 | 38.84 | 39.25 | 39.01 | 38.73 | 38.87 | 39.27 | 38.93 | 38.76 | 38.63 | MR |
| $n_D$ | 1.3974 | 1.3949 | 1.4002 | 1.3979 | 1.4018 | 1.3925 | 1.3929 | 1.4011 | 1.4041 | 1.404 | 1.3935 | 1.4001 | 1.4078 | 1.4042 | 1.3915 | 1.403 | 1.4075 | 1.4695 | $n_D$ |
| BP/Tc | 0.7012 | 0.6984 | 0.6957 | 0.6959 | 0.6927 | 0.6950 | 0.6913 | 0.6900 | 0.6872 | 0.6857 | 0.6911 | 0.6853 | 0.6789 | 0.6827 | 0.6847 | 0.6797 | 0.6764 | 0.6685 | BP/Tc |
| $Tc^2/Pc$ | 129822 | 126113 | 124807 | 124162 | 122619 | 121677 | 119903 | 120827 | 119914 | 119112 | 119569 | 119049 | 118400 | 117553 | 115240 | 116312 | 116673 | 112333 | $Tc^2/Pc$ |
| Tc/Pc | 228.20 | 225.32 | 221.41 | 221.01 | 216.83 | 221.19 | 216.59 | 214.42 | 210.78 | 210.04 | 217.44 | 211.79 | 205.34 | 207.51 | 211.84 | 206.41 | 203.40 | 197.84 | Tc/Pc |
| CED | 0.05058 | 0.04937 | 0.05005 | 0.04996 | 0.05016 | 0.04735 | 0.04776 | 0.04950 | 0.05011 | 0.04962 | 0.04693 | 0.04823 | 0.04992 | 0.04923 | 0.04488 | 0.04796 | 0.04914 | 0.05418 | CED |
| Sol.par. | 0.2249 | 0.2222 | 0.2237 | 0.2235 | 0.2240 | 0.2176 | 0.2185 | 0.2225 | 0.2238 | 0.2228 | 0.2166 | 0.2196 | 0.2234 | 0.2219 | 0.2119 | 0.2190 | 0.2217 | 0.2328 | Sol.par. |
| ΔHv | 8.225 | 8.08 | 8.1 | 8.1 | 8.03 | 7.8 | 7.79 | 7.94 | 7.95 | 7.88 | 7.71 | 7.76 | 7.84 | 7.82 | 7.41 | 7.65 | 7.73 | 7.51 | ΔHv |
| ΔHf°g | 49.82 | 51.5 | 50.82 | 50.69 | 50.38 | 53.21 | 52.44 | 51.13 | 50.91 | 50.48 | 53.71 | 52.61 | 51.38 | 51.97 | 53.57 | 52.61 | 51.73 | 53.99 | ΔHf°g |
| ω | 0.398 | 0.378 | 0.37 | 0.371 | 0.361 | 0.356 | 0.343 | 0.346 | 0.338 | 0.33 | 0.338 | 0.32 | 0.303 | 0.315 | 0.303 | 0.297 | 0.29 | 0.251 | ω |
| BP | 398.805 | 390.797 | 392.075 | 390.859 | 391.684 | 382.253 | 382.579 | 388.757 | 390.875 | 388.8 | 379.99 | 385.119 | 391.409 | 386.617 | 372.388 | 382.99 | 387.91 | 379.62 | BP |
| d | 0.7025 | 0.698 | 0.7058 | 0.7046 | 0.7136 | 0.6935 | 0.7004 | 0.7121 | 0.72 | 0.7193 | 0.6953 | 0.71 | 0.7274 | 0.7191 | 0.6919 | 0.7161 | 0.7262 | 0.8242 | d |
| Vm | 162.61 | 163.66 | 161.85 | 162.12 | 160.08 | 164.72 | 163.1 | 160.42 | 158.66 | 158.81 | 164.29 | 160.89 | 157.04 | 158.85 | 165.1 | 159.52 | 157.3 | 138.6 | Vm |
| logVP | 3.28 | 3.31 | 3.49 | 3.31 | 3.32 | 3.57 | 3.89 | 3.54 | 3.33 | 3.56 | 3.57 | 3.64 | 3.49 | 3.55 | 3.8 | 3.63 | 3.55 | | logVP |
| Tc | 568.76 | 559.57 | 563.6 | 561.67 | 565.42 | 549.99 | 553.45 | 563.42 | 568.78 | 567.02 | 549.8 | 561.95 | 576.51 | 566.34 | 543.89 | 563.43 | 573.49 | 567.85 | Tc |
| Pc | 24.54 | 24.52 | 25.13 | 25.09 | 25.74 | 24.54 | 25.23 | 25.94 | 26.57 | 26.65 | 24.76 | 26.19 | 27.71 | 26.94 | 25.43 | 26.94 | 27.83 | 28.3 | Pc |
| dc | 0.232 | 0.234 | 0.246 | 0.24 | 0.251 | 0.237 | 0.242 | 0.244 | 0.245 | 0.258 | 0.239 | 0.258 | 0.251 | 0.248 | 0.244 | 0.262 | 0.251 | 0.248 | dc |
| Vc | 0.4924 | 0.4882 | 0.4644 | 0.476 | 0.4551 | 0.482 | 0.4721 | 0.4682 | 0.4663 | 0.4428 | 0.478 | 0.4428 | 0.4551 | 0.4606 | 0.4682 | 0.436 | 0.4551 | 0.4606 | Vc |
| Zc | 0.259 | 0.261 | 0.252 | 0.259 | 0.252 | 0.262 | 0.262 | 0.263 | 0.265 | 0.254 | 0.264 | 0.251 | 0.267 | 0.267 | 0.266 | 0.254 | 0.269 | 0.28 | Zc |
| αc | 7.76 | 7.68 | 7.58 | 7.58 | 7.58 | 7.5 | 7.47 | 7.47 | 7.4 | 7.47 | 7.49 | 7.48 | 7.32 | 7.35 | 7.37 | 7.25 | 7.28 | 7.65 | αc |
| A | 6.919 | 6.917 | 6.899 | 6.901 | 6.891 | 6.86 | 6.853 | 6.87 | 6.88 | 6.867 | 6.837 | 6.851 | 6.867 | 6.854 | 6.812 | 6.825 | 6.844 | 6.877 | A |
| B | 1351.99 | 1337.47 | 1331.53 | 1327.66 | 1327.88 | 1287.27 | 1287.88 | 1315.5 | 1330.04 | 1318.12 | 1273.59 | 1307.88 | 1347 | 1315.08 | 1257.84 | 1294.88 | 1328.05 | 1329.93 | B |
| C | 209.15 | 213.69 | 212.41 | 212.57 | 212.6 | 214.41 | 214.79 | 214.16 | 214.86 | 215.31 | 215.07 | 217.44 | 219.68 | 217.53 | 220.74 | 218.42 | 220.38 | 226.36 | C |
| PCP \ Octane | Oct | 2M7 | 3M7 | 4M7 | 3Et6 | 25M6 | 24M6 | 23M6 | 34M6 | 3Et2M5 | 22M6 | 33M6 | 3Et3M5 | 234M5 | 224M5 | 223M5 | 233M5 | 2233M4 | Octane \ PCP |

The data for the boiling point (BP), density (d), the critical data Tc, Pc, Vc, Zc, αc, and dc, the standard enthalpy of formation for the ideal gas (ΔHf°g), the enthalpy of vaporisation (ΔHv), the Antoine constants A, B, and C, as well as the Pitzer's acentric factor (ω) and the refractive index ($n_D$) were taken from the CRC Handbook[1] or from Lange's Handbook[2]. The data for the liquid molar volume (Vm), the ratios $Tc^2/Pc$ and Tc/Pc used instead of the van der Waals parameters $a_0$ and $b_0$, the ratio BP/Tc (reduced BP), the molar refraction (MR), cohesive energy density (CED) and its square root, the solubility parameter (Sol. par.) were calculated from data presented in the handbooks. The data for Octane Numbers (BON, MON, RON) were taken from: Pogliani,[3] Balaban and Motoc,[4] Gutman et al.,[5] Warnatz et al.,[6] and Morley;[7] those for vapour pressure (logVP) from Goll and Jurs,[8] and those for the entropy (S) and quadratic mean radius ($R^2$) from Ren.[9] Surface tension (ST) data were taken from Li.[10]

**References A1.**


1. D. R. Lide, CRC Handbook of Chemistry and Physics, 76th Ed., CRC Press, Boca Raton 1995-96.
2. J. A. Dean, Lange's Handbook of Chemistry, McGraw-Hill, New York 1985.
3. L. Pogliani, J. Phys. Chem. 1995, 99, 925-937.
4. A. T. Balaban, I. Motoc, MATCH (Commun. Math. Chem.) 1979, 5, 197-218.
5. I. Gutman, W. Linert, I. Lukovits, Z. Tomović, J. Chem. Inf. Comput. Sci. 2000, 40, 113-143.
6. J. Warnatz, Combustion: physical and chemical fundamentals, modeling and simulation, experiments, pollutants formation, J. Warnatz, U. Maas, R.W. Dibble, 2nd Ed., Springer, Berlin etc 1999.
7. C. Morley, Combust. Sci., Technol. 1987, 55, 115-123.
8. E. S. Goll, P.C. Jurs, J. Chem. Inf. Comput. Sci. 1999, 39, 1081-1089.
9. B. Ren, J. Chem. Inf. Comput. Sci. 1999, 39, 139-143.
10. X. H. Li, Chem. Phys. Lett. 2002, 365, 135-139.