

Thermodynamic Properties of Light Synthetic Natural Gas Mixtures

Using the RK–PR Cubic Equation of State

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Supporting Information

Table S1. Binary systems literature data for the correlation of interaction parameters. For each pair we report the temperature range (K), number of data points (parenthesized) and [reference]^a

Methane		Ethane	Propane	i-Butane	n-Butane	i-Pentane	n-Pentane	n-Hexane	n-Heptane	n-Octane	Nitrogen
Methane	—	—	—	—	—	—	—	—	—	—	—
Ethane	130.37 – 283.15 (90) [1,2,3]	—	—	—	—	—	—	—	—	—	—
Propane	158.15 – 344.26 (98) [4,5]	255.37 – 355.37 (49) [18]	—	—	—	—	—	—	—	—	—
i-Butane	310.93 – 377.59 (41) [6]	311.26 – 394.04 (40) [19]	266.54 – 394.26 (78) [28]	—	—	—	—	—	—	—	—
n-Butane	166.48 – 360.93 (86) [7,8]	338.71 – 394.26 (19) [20]	333.15 – 413.15 (22) [29]	273.15 (22) [39]	—	—	—	—	—	—	—
i-Pentane	344.26 – 444.26 (19) [9]	*	273.15 – 423.15 (82) [30]	*	*	—	n-Pentane	—	—	—	—
n-Pentane	176.21 – 377.59 (95) [10,11]	277.59 – 444.26 (74) [21]	344.26 – 427.59 (69) [31]	*	298.15 (12) [43]	*	—	n-Hexane	—	—	—
n-Hexane	183.15 – 423.15 (60) [12]	338.71 – 449.82 (32) [22]	333.15 – 433.15 (32) [32]	*	*	*	298.15 – 337.35 (50) [49-51]	—	n-Heptane	—	—
n-Heptane	277.59 – 410.93 (76) [13]	338.71 – 449.82 (62) [23]	333.15 – 433.15 (26) [33]	*	*	*	403.71 – 526.45 (42) [51-53]	—	—	n-Octane	—
n-Octane	223.15 – 423.15 (49) [14]	273.15 – 373.15 (51) [24]	273.15 – 373.15 (78) [34,35]	*	*	*	291.52 – 433.63 (94) [51]	388.35 – 388.35 (75) [57-59]	313.85 – 394.45 (89) [57,58,62,6 2,1]	—	Nitrogen
Nitrogen	133.71 – 183.15 (68) [15]	138.71 – 290.00 (74) [25,26]	143.15 – 290.00 (55) [26,36]	255.37 – 394.26 (52) [40]	310.93 – 410.93 (28) [44]	277.59 – 377.37 (47) [47]	277.43 – 377.59 (42) [54]	310.93 – 444.26 (52) [60]	305.37 – 455.37 (34) [64]	322.00 – 344.00 (12) [66]	—
Carbon Dioxide	183.25 – 271.48 (56) [16,17]	223.15 – 293.15 (65) [27]	233.15 – 344.26 (81) [37,38]	273.15 – 394.26 (53) [41,42]	227.98 – 377.59 (73) [45,46]	277.59 – 377.65 (46) [48]	277.65 – 377.59 (53) [55]	298.15 – 313.15 (20) [61]	310.65 – 477.21 (64) [65]	*	218.15 – 293.15 (35) [67,68]

^aReferences for Table S1:

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* Isothermal VLE data not available.

Table S2. Correlation results for binary vapor – liquid equilibrium with RK – PR equation of state and one-fluid mixing rule. For each binary system, binary interaction parameter, and (AAD (K_1) – AAD (K_2)), eq. 9, are reported

Methane		Ethane		Propane		i-Butane		n-Butane		i-Pentane		n-Pentane		n-Hexane		n-Heptane		n-Octane		Nitrogen						
Methane	—																									
Ethane	-0.0001 (1.42 - 2.15)	—																								
Propane	0.0062 (0.24 - 1.01)	-0.0017 (1.47 - 2.11)	—																							
i-Butane	-0.0110 (0.34 - 0.39)	-0.0143 (1.18 - 3.02)	0.0040 (0.60 - 1.19)																							
n-Butane	-0.0037 (0.96 - 1.99)	-0.0332 (0.43 - 0.30)	-0.0051 (0.57 - 0.90)	0.0020 (0.15 - 0.44)																						
i-Pentane	0.0063 (2.11 - 0.61)	*	0.0032 (3.62 - 3.72)	*																						
n-Pentane	0.0102 (0.66 - 1.41)	0.0028 (0.98 - 4.54)	0.0036 (4.32 - 4.15)	*	-0.0070 (2.92 - 0.57)																					
n-Hexane	-0.0043 (1.05 - 2.89)	-0.0075 (3.46 - 5.48)	-0.0057 (0.58 - 2.49)	*	*																					
n-Heptane	0.0020 (0.66 - 1.41)	-0.0282 (2.49 - 4.90)	0.0318 (0.42 - 4.25)	*	*																					
n-Octane	-0.0305 (4.11 - 3.00)	0.0329 (1.18 - 5.54)	0.0381 (1.09 - 4.54)	*	*																					
Nitrogen	-0.0021 (1.62 - 3.82)	-0.0016 (3.58 - 7.09)	-0.0256 (3.13 - 4.27)	-0.0209 (3.67 - 6.65)	-0.0079 (0.59 - 1.22)	-0.0314 (7.65 - 2.75)																				
Carbon Dioxide	-0.0340 (3.46 - 4.48)	-0.0210 (3.90 - 4.79)	-0.0038 (2.85 - 6.12)	0.0078 (3.48 - 6.02)	-0.0036 (3.05 - 6.04)	-0.0155 (2.95 - 8.06)	-0.0146 (7.19 - 5.61)	-0.0152 (2.48 - 3.93)	-0.0194 (5.52 - 7.27)	-0.0102 (3.06 - 2.25)	0.0251 (1.52 - 4.14)	-0.0087 (1.48 - 2.05)	0.0219 (0.72 - 4.03)	-0.0058 (2.81 - 0.47)	0.0027 (0.52 - 1.14)	-0.0379 (6.88 - 5.81)	-0.0405 (7.05 - 6.21)	0.0057 (1.41 - 0.57)								