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PYTHON-BASED CALCULATION OF FOUR KEY THERMODYNAMIC PARAMETERS FOR EIGHT ALKANES

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ABSTRACT

In modern era, lower alkanes n-C_xH_{2x+2} (where x ranges from 1 to 8) are vital fuels owing to their inertness and favorable combustion properties. Understanding the thermodynamic properties becomes crucial. This article presents Python code to calculate four key thermodynamic parameters for eight alkanes over a temperature range of 298 to 1498 kelvin. We have investigated the variation of heat capacity with temperature using temperature dependent C_p equation, visualized through C_p *Vs* T plots. These C_p values are then employed to determine changes in enthalpies using Kirchhoff's equation. Using the third law of thermodynamics, entropy changes are also computed. To explore temperature-dependent variations, ΔH *Vs* T and ΔS *Vs* T graphs are plotted. Finally, Gibbs free energy changes (ΔG) are derived using ΔH and ΔS values and plotted against different temperatures, offering valuable insights into the thermodynamic behavior of lower alkanes.

Keywords: Heat capacity, Enthalpy change, Entropy Change, Gibbs free energy, temperature-dependent variations, Python

1. INTRODUCTION

Lower alkanes, methane and ethane are the main components of Compressed Natural Gas (CNG); however, propane and butane are major components of Liquified Petroleum Gas (LPG). Alkanes from pentane to octane are utilized as fuels for internal combustion engines[1]. Studying the thermodynamic properties[2,3] of these alkanes is essential to analyse the energy dynamics involved in chemical reactions including oxidation. Thermodynamic quantities such as heat capacity, change in enthalpy, entropy and free energy provide insights into energy changes, phase transitions and reaction spontaneity, aiding advancements in quantum chemistry[4], surface chemistry[5] and material design.

Despite the importance, calculation of various thermodynamic parameters is time-consuming task due to complexity of the equations involved. Over the years, many computational programs[6–9] and toolbox[10–12,13] have been developed to ease these calculations. For example, B. J. McBride and associates[14] derived PAC91 program for ideal gases and other gases. Python[15] has emerged as a valuable tool for due to its flexibility, ease of debugging and extensive libraries.

This article presents Python code to calculate C_p, ΔH, ΔS and ΔG for eight alkanes n-C_xH_{2x+2} (x=1 to 8) over a temperature range of 298 to 1498 kelvin, offering an efficient approach to thermodynamic analysis.

2. Programming details

2.1 Variation of the Heat Capacity with Temperature at Constant Pressure

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The Shomate equation[16] describes the variation of heat capacity with temperature at constant pressure:

$$C_P = A + BT + CT^2 + DT^{-2}$$

The A, B, C… are the coefficients characteristic to each substance. In this study, we calculated C_p for eight alkanes n-C_xH_{2x+2} (x=1 to 8) for temperature range 298 to 1498 kelvin using the modified form:

$$\frac{C_p}{R} = A + BT + CT^2 + DT^{-2} \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Here, R = 8.314 J K^{-1} mol^{-1} is universal gas constant. The coefficients A, B, C… are independent of temperature but are pressure dependent. For ideal gas situation, values for these coefficients are obtained from literature for methane, ethane, n-propane, n-butane, n-pentane, n-hexane, n-heptane and n-octane[17]. For methane gas values of A = 1.702, B = 9.081×10^{-3} and C = -2.164×10^{-6}, D is usually zero, depending on the substance under consideration. Substituting these values in equation (1) gives:

$$\frac{C_p}{8.314} = 1.702 + 9.081\times10^{-3}T - 2.164\times10^{-6}T^2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

$$C_p = 8.314\times1.702 + 8.314\times9.081\times10^{-3}T - 8.314\times2.164\times10^{-6}T^2 \ldots\ldots\ldots\ldots\ldots\ldots (3)$$

$$C_p = 14.15 + 0.075499\,T - 0.00001799\,T^2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

Python code 2.1.1 is developed using equation (4) to calculate and plot the variation of C_p of methane over the temperature range 298 to 1498 K.

2.1.1 Python Code for Heat Capacity C_p Calculation and Graph C_p Vs T

```
import numpy as np
import matplotlib.pyplot as plt
# Constants
R = 8.314
a = 1.702
b = 9.081 * 10**-3
c = -2.164 * 10**-6
# Temperature range
T_values = np.arange(298, 1499, 50)
# Calculate Cp for each temperature
Cp_values = R * a + R * b * T_values + R * c * T_values**2
# Plotting
plt.plot(T_values, Cp_values, color='red',label='Methane', linestyle="-", markersize=7, marker='v')
plt.xlabel('Temperature (K)')
plt.ylabel('Cp(J/K)')
plt.grid(True)
plt.legend()
plt.show()
# Printing table
print("Temperature (K)\t Cp")
for T, Cp in zip(T_values, Cp_values):
   print(f"{T}\t\t {Cp}")
```

This code is adaptable for other alkanes by adjusting A, B and C for each alkane. The C_p equations for other alkanes are also written here, using their corresponding A, B and C as listed in Table 1

For Ethane; $C_p = 9.40 + 0.1599\,T - 0.0000462341\,T^2$

For Propane; $C_p = 10.08 + 0.2390\,T - 0.00007336\,T^2$

For *n*-Butane; $C_p = 16.08 + 0.3069\,T - 0.00009479\,T^2$

For *n*-Pentane; $C_p = 20.48 + 0.3370\,T - 0.00011731\,T^2$

For *n*-Hexane; $C_p = 25.15 + 0.4464\,T - 0.00013960\,T^2$

For *n*-Heptane; $C_p = 29.68 + 0.5160\,T - 0.00016200\,T^2$

For *n*-Octane; $C_p = 34.15 + 0.5860\,T - 0.00018400\,T^2$

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The calculated values of heat capacity C_p for all eight alkanes, obtained using Python code **2.1.1,** are presented in Table 2. Although the output graphs of C_p Vs temperature from Python code **2.1.1** are not shown here, an additional python script **2.1.2** is developed to plot a graph C_p Vs temperature (Figure 1) for eight alkanes enabling better comparison.

2.1.2 Python Code to Plot C_p Vs T for Eight Alkanes

```
import matplotlib.pyplot as plt
# Data
temperatures = [298, 348, 398, 448, 498, 548, 598, 648, 698, 748, 798, 848, 898, 948, 998, 1048, 1098, 1148, 1198, 1248, 1298, 1348, 1398, 1448, 1498]
# Heat Capacity data for different gases
methane = [35.05, 38.25, 41.35, 44.36, 47.29, 50.12, 52.87, 55.52, 58.08, 60.56, 62.94, 65.24, 67.44, 69.55, 71.58, 73.51, 75.36, 77.11, 78.78, 80.35, 81.84, 83.23, 84.54, 85.75, 86.88]
ethane = [52.93, 59.43, 65.69, 71.73, 77.54, 83.11, 88.45, 93.56, 98.44, 103.09, 107.51, 111.7, 115.65, 119.38, 122.87, 126.13, 129.16, 131.96, 134.53, 136.87, 138.98, 140.85, 142.49, 143.91, 145.09]
propane = [74.89, 84.48, 93.71, 102.58, 111.07, 119.2, 126.96, 134.36, 141.39, 148.05, 154.34, 160.27, 165.83, 171.03, 175.86, 180.32, 184.41, 188.14, 191.49, 194.49, 197.11, 199.37, 201.27, 202.79, 203.95]
n_butane = [99.13, 111.41, 123.22, 134.56, 145.42, 155.81, 165.72, 175.16, 184.13, 192.62, 200.64, 208.18, 215.25, 221.85, 227.97, 233.62, 238.79, 243.49, 247.72, 251.47, 254.75, 257.55, 259.88, 261.74, 263.12]
n_pentane = [122.43, 137.49, 151.97, 165.86, 179.16, 191.88, 204.01, 215.55, 226.51, 236.88, 246.66, 255.86, 264.47, 272.49, 279.93, 286.78, 293.04, 298.72, 303.81, 308.32, 312.24, 315.57, 318.31, 320.47, 322.04]
n_hexane = [145.85, 163.68, 180.8, 197.23, 212.96, 227.99, 242.32, 255.96, 268.89, 281.13, 292.67, 303.52, 313.66, 323.11, 331.86, 339.91, 347.26, 353.92, 359.88, 365.13, 369.7, 373.56, 376.72, 379.19, 380.96]
n_heptane = [169.22, 189.81, 209.59, 228.57, 246.73, 264.08, 280.63, 296.36, 311.28, 325.4, 338.7, 351.19, 362.88, 373.75, 383.81, 393.07, 401.51, 409.14, 415.96, 421.98, 427.18, 431.57, 435.16, 437.93, 439.89]
n_octane = [192.59, 215.96, 238.41, 259.94, 280.54, 300.21, 318.97, 336.8, 353.71, 369.7, 384.76, 398.9, 412.11, 424.41, 435.78, 446.22, 455.74, 464.34, 472.02, 478.77, 484.61, 489.51, 493.5, 496.56, 498.69]
# Markers and colors
markers = ['o', '^', 'h', 'd','X','p','v', '*']
colors = ['red', 'Blue','green', 'Purple', 'Orange', 'Brown','Magenta', 'olive']
labels = ['Methane', 'Ethane', 'Propane', 'nButane', 'nPentane', 'nHexane','nHeptane','nOctane']
# Plotting
plt.figure(figsize=(10, 6))
for i, gas in enumerate([methane, ethane, propane, n_butane, n_pentane, n_hexane, n_heptane, n_octane]):
    plt.plot(temperatures, gas, marker=markers[i], color=colors[i],linestyle='--', label=labels[i], markersize=8)

plt.xlabel('Temperature (K)', fontsize=16)
plt.ylabel(' Heat Capacity Cp (J/K)', fontsize=16)
plt.xticks(fontsize=12)  # Increase font size for x axis tick marks
plt.yticks(fontsize=12)  # Increase font size for y axis tick marks
plt.legend( fontsize=10)  # Add legend for clarity
plt.show()
```

Table 1: Values of A, B and C for the Alkanes[17] and Standard Enthalpies of Formation at 298.15 K[18,19]

Alkane	A	B × 10^3	C × 10^6	$\Delta H_f^o{}_{298}$ (J/mol)
Methane (CH_4)	1.702	9.081	−2.164	−74520
Ethane (C_2H_6)	1.131	19.225	−5.561	−83820
Propane (C_3H_8)	1.213	28.785	−8.824	−104680
n-Butane (C_4H_{10})	1.935	36.915	−11.402	−125790
n-Pentane (C_5H_{12})	2.464	45.351	−14.111	−146760
n-Hexane (C_6H_{14})	3.025	53.722	−16.791	−166920
n-Heptane (C_7H_{16})	3.570	62.127	−19.486	−187780
n-Octane (C_8H_{18})	4.108	70.567	−22.208	−208750

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Table 2: Values of Heat Capacity, C_p ($J\,K^{-1}$) for Methane, Ethane, *n*-Propane, *n*-Butane, *n*-Pentane, *n*-Hexane, *n*-Heptane and *n*-Octane

S. No.	T*(K)	Heat Capacity C_p ($J\,K^{-1}$)							
		CH_4	C_2H_6	*n*-C_3H_8	*n*-C_4H_{10}	*n*-C_5H_{12}	*n*-C_6H_{14}	*n*-C_7H_{16}	n-C_8H_{18}
1	298	35.05	52.93	74.89	99.13	122.43	145.85	169.22	192.59
2	348	38.25	59.43	84.48	111.41	137.49	163.68	189.81	215.96
3	398	41.35	65.69	93.71	123.22	151.97	180.80	209.59	238.41
4	448	44.36	71.73	102.58	134.56	165.86	197.23	228.57	259.94
5	498	47.29	77.54	111.07	145.42	179.16	212.96	246.73	280.54
6	548	50.12	83.11	119.2	155.81	191.88	227.99	264.08	300.21
7	598	52.87	88.45	126.96	165.72	204.01	242.32	280.63	318.97
8	648	55.52	93.56	134.36	175.16	215.55	255.96	296.36	336.80
9	698	58.08	98.44	141.39	184.13	226.51	268.89	311.28	353.71
10	748	60.56	103.09	148.05	192.62	236.88	281.13	325.40	369.70
11	798	62.94	107.51	154.34	200.64	246.66	292.67	338.70	384.76
12	848	65.24	111.7	160.27	208.18	255.86	303.52	351.19	398.90
13	898	67.44	115.65	165.83	215.25	264.47	313.66	362.88	412.11
14	948	69.55	119.38	171.03	221.85	272.49	323.11	373.75	424.41
15	998	71.58	122.87	175.86	227.97	279.93	331.86	383.81	435.78
16	1048	73.51	126.13	180.32	233.62	286.78	339.91	393.07	446.22
17	1098	75.36	129.16	184.41	238.79	293.04	347.26	401.51	455.74
18	1148	77.11	131.96	188.14	243.49	298.72	353.92	409.14	464.34
19	1198	78.78	134.53	191.49	247.72	303.81	359.88	415.96	472.02
20	1248	80.35	136.87	194.49	251.47	308.32	365.13	421.98	478.77
21	1298	81.84	138.98	197.11	254.75	312.24	369.70	427.18	484.61
22	1348	83.23	140.85	199.37	257.55	315.57	373.56	431.57	489.51
23	1398	84.54	142.49	201.27	259.88	318.31	376.72	435.16	493.50
24	1448	85.75	143.91	202.79	261.74	320.47	379.19	437.93	496.56
25	1498	86.88	145.09	203.95	263.12	322.04	380.96	439.89	498.69

T* = Temperature

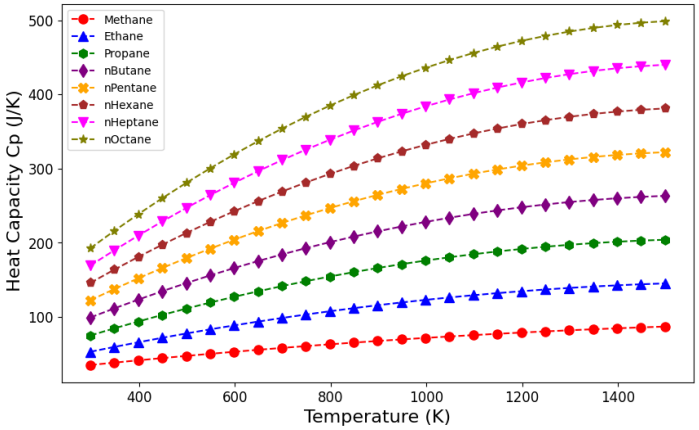

Figure 1: Heat Capacity, Cp Vs Temperature

From the values C_p in Table 2 and the trends illustrated in Figure 1, it is evident that C_p increases with rise in temperature for all alkanes. This increase is more pronounced in higher alkanes at elevated temperatures. This suggests that lower alkanes are more efficient fuels compared to higher ones as they require less heat to raise the temperature by 1 K. For instance, methane requires 35.05 J energy at 298 K and 86.88 J at 1498 K to raise the temperature by 1 K, resulting in a difference of 51.83 J. In contrast, n-octane shows more significant difference of 305.41 J for the same temperatures

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difference. The plots (Figure 1) indicate that heat capacity of all alkanes increases almost linearly with temperature. However, a deviation from linearity is observed beyond 800 K in all alkanes becoming more pronounced at higher temperatures, especially for higher alkanes.

2.2 Entropy Change Calculations

From third law of thermodynamics, entropy of a system can be given by:

$$\Delta S = \int_{T_1}^{T_2} \frac{C_P}{T} dT \dots\dots\dots\dots\dots (5)$$

Putting the value of C_p in equation (5) from equation (4):

$$\Delta S = \int_{T_1}^{T_2} \frac{14.15 + 75.499 \times 10^{-3} T - 17.99 \times 10^{-6} T^2}{T} dT \dots\dots\dots\dots\dots (6)$$

$$\Delta S = \int_{T_1}^{T_2} \frac{14.15}{T} dT + \int_{T_1}^{T_2} 75.499 \times 10^{-3} dT - \int_{T_1}^{T_2} 17.99 \times 10^{-6}\, T dT \dots\dots\dots (7)$$

$$\Delta S = 14.15 \ln \frac{T_2}{T_1} + 75.499\,(T_2 - T_1) - \frac{17.99}{2}(T_2^2 - T_1^2) \dots\dots\dots\dots\dots (8)$$

The equation (5) is solved for methane gas only; same calculations can be used for other gases. Herein we have written python code for calculating ΔS for eight alkanes n-C_xH_{2x+2} (x=1 to 8) for temperature range 298 to 1498 kelvin using the equation (8).

2.2.1 Python Code for Entropy Change (ΔS) Calculation and Graph ΔS Vs T

```
import sympy as sp
import numpy as np
import matplotlib.pyplot as plt
# Constants
A = 14.150428
B = 0.075499434
C = -0.000017991496
# Symbolic variable
T_sym = sp.symbols('T')
# Define integrands
integrand_A = A / T_sym
integrand_B = B
integrand_C = 0.5 * C * (T_sym**2)
# Perform symbolic integration with limits
integral_A = sp.integrate(integrand_A, (T_sym, 298, 348))
integral_B = sp.integrate(integrand_B, (T_sym, 298, 348))
integral_C = sp.integrate(integrand_C, (T_sym, 298, 348))
# Evaluate delS for each component
delS_A = integral_A
delS_B = integral_B * (348 - 298)  # Interval: 50
delS_C = integral_C
# Initialize variables
lower_limit = 298
upper_limit = 1498
interval = 50
# Initialize lists to store T values and corresponding delS values
T_values = []
delS_values = []
# Loop through the range of T values
T = lower_limit
while T <= upper_limit:
    # Calculate delS for the current T value
    delS_A = A * (np.log(T) - np.log(lower_limit))
    delS_B = B * (T - lower_limit)
    delS_C = 0.5 * C * (T**2 - lower_limit**2)
```

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```
    delS = delS_A + delS_B + delS_C
    # Append T value and delS value to the lists
    T_values.append(T)
    delS_values.append(delS)
    # Print the calculated delS values for the current T value
    print(f"T = {T}, delS = {delS}")
    # Increment T by 50
    T += interval
# Plot the graph with colorful lines and marker style square
for i in range(len(T_values) - 1):
    color = plt.cm.viridis(i / len(T_values))  # Using a colormap to generate colors
    plt.plot(T_values[i:i+2], delS_values[i:i+2], color='red', label='Integral Values', marker='p', markersize=10,
linestyle='-')
plt.xlabel('Temperature (K)')
plt.legend(['Methane'], loc='upper left')
plt.ylabel('Entropy Change ΔS (J/K)')
plt.grid(True)
plt.show()
```

The output of Python code **2.2.1** provides entropy ΔS values for methane gas over a temperature range of 298 to 1498 K along with a plot for ΔS versus T. The same code can used to calculate ΔS for other alkanes by simply changing variables A, B and C for each alkane.

Table 3: Values of Entropy change, ΔS ($J\,K^{-1}$) for Methane, Ethane, *n*-Propane, *n*-Butane, *n*-Pentane, *n*-Hexane, *n*-Heptane and *n*-Octane

S. No.	T (K)	Entropy change ΔS (JK^{-1})							
		CH_4	C_2H_6	*n*-C_3H_8	*n*-C_4H_{10}	*n*-C_5H_{12}	*n*-C_6H_{14}	*n*-C_7H_{16}	*n*-C_8H_{18}
1	298	-	-	-	-	-	-	-	-
2	348	5.68	8.70	12.35	16.31	20.14	23.98	27.81	31.65
3	398	11.02	17.10	24.30	32.05	39.55	47.08	54.60	62.13
4	448	16.09	25.22	35.90	47.29	58.35	69.44	80.52	91.60
5	498	20.93	33.12	47.20	62.10	76.59	91.13	105.65	120.18
6	548	25.59	40.80	58.22	76.50	94.34	112.22	130.08	147.95
7	598	30.09	48.29	68.96	90.54	111.62	132.75	153.86	174.98
8	648	34.44	55.59	79.45	104.22	128.46	152.75	177.02	201.31
9	698	38.66	62.73	89.70	117.57	144.89	172.26	199.60	226.97
10	748	42.76	69.70	99.71	130.61	160.91	191.28	221.62	251.99
11	798	46.76	76.51	109.49	143.33	176.56	209.84	243.11	276.40
12	848	50.65	83.17	119.05	155.75	191.83	227.96	264.07	300.21
13	898	54.45	89.69	128.39	167.88	206.73	245.64	284.53	323.44
14	948	58.16	96.05	137.52	179.72	221.28	262.89	304.48	346.11
15	998	61.79	102.28	146.43	191.28	235.48	279.73	323.95	368.21
16	1048	65.34	108.37	155.14	202.57	249.33	296.15	342.95	389.77
17	1098	68.81	114.32	163.64	213.58	262.84	312.16	361.46	410.80
18	1148	72.20	120.13	171.94	224.31	276.02	327.78	379.51	431.28
19	1198	75.53	125.81	180.03	234.79	288.87	342.99	397.10	451.25
20	1248	78.78	131.36	187.92	244.99	301.38	357.82	414.24	470.69
21	1298	81.96	136.78	195.61	254.94	313.57	372.25	430.92	489.61
22	1348	85.08	142.07	203.11	264.62	325.44	386.30	447.15	508.02
23	1398	88.14	147.23	210.41	274.04	336.98	399.96	462.93	525.93
24	1448	91.13	152.26	217.51	283.21	348.21	413.25	478.28	543.32
25	1498	94.06	157.17	224.41	292.12	359.12	426.15	493.18	560.22

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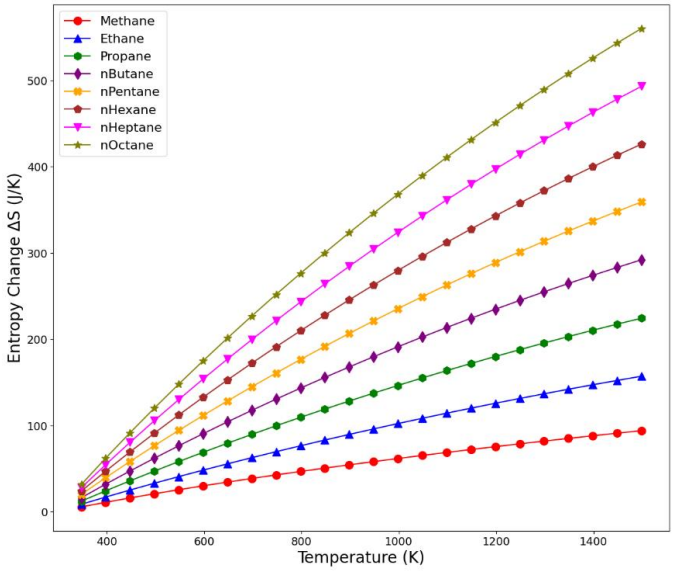

Figure 2: Entropy, ΔS Vs Temperature

The calculated values of ΔS for all eight alkanes using Python code **2.2.1** are listed in table 3. Although individual ΔS Vs temperature graphs from this code are not presented here, an extra script Python code **2.2.2** is created to generate combined plot of ΔS Vs temperature (Figure 2) for all alkanes, like C_p Vs temperature. It is clear from data in table 3 and figure 2 that ΔS increases with temperature from 298 K to 1498 K for all the alkanes. This increase in ΔS indicates an increase in thermal energy leading to greater disorder as temperature rises. This effect becomes more prominent at higher temperatures, resulting the enhanced molecular motion and increased randomness within the system. This trend is particularly notable in higher alkanes such as n-octane, where the difference in ΔS from 348 K to 1498 K is 528.57 K (ΔS_{1498}- ΔS_{348}= 528.57) compared to lower alkanes viz. methane which shows an increase of only 88.38 K (ΔS_{1498}- ΔS_{348}= 88.38) in the same temperature range. This greater increase in ΔS can be attributed to their large molecular size. Large molecules experience more collisions leading to increased randomness and thus a greater increase in entropy with rise in temperature.

2.2.2 Python Code to Plot ΔS Vs T for Eight Alkanes

```
import matplotlib.pyplot as plt# Data
temperature = [298, 348, 398, 448, 498, 548, 598, 648, 698, 748, 798, 848, 898, 948, 998, 1048, 1098, 1148, 1198, 1248, 1298, 1348, 1398, 1448, 1498]
CH4 = [None, 5.68, 11.02, 16.09, 20.93, 25.59, 30.09, 34.44, 38.66, 42.76, 46.76, 50.65, 54.45, 58.16, 61.79, 65.34, 68.81, 72.20, 75.53, 78.78, 81.96, 85.08, 88.14, 91.13, 94.06]
C2H6 = [None, 8.70, 17.10, 25.22, 33.12, 40.80, 48.29, 55.59, 62.73, 69.70, 76.51, 83.17, 89.69, 96.05, 102.28, 108.37, 114.32, 120.13, 125.81, 131.36, 136.78, 142.07, 147.23, 152.26, 157.17]
C3H8 = [None, 12.35, 24.30, 35.90, 47.20, 58.22, 68.96, 79.45, 89.70, 99.71, 109.49, 119.05, 128.39, 137.52, 146.43, 155.14, 163.64, 171.94, 180.03, 187.92, 195.61, 203.11, 210.41, 217.51, 224.41]
C4H10 = [None, 16.31, 32.05, 47.29, 62.10, 76.50, 90.54, 104.22, 117.57, 130.61, 143.33, 155.75, 167.88, 179.72, 191.28, 202.57, 213.58, 224.31, 234.79, 244.99, 254.94, 264.62, 274.04, 283.21, 292.12]
C5H12 = [None, 20.14, 39.55, 58.35, 76.59, 94.34, 111.62, 128.46, 144.89, 160.91, 176.56, 191.83, 206.73, 221.28, 235.48, 249.33, 262.84, 276.02, 288.87, 301.38, 313.57, 325.44, 336.98, 348.21, 359.12]
C6H14 = [None, 23.98, 47.08, 69.44, 91.13, 112.22, 132.75, 152.75, 172.26, 191.28, 209.84, 227.96, 245.64, 262.89, 279.73, 296.15, 312.16, 327.78, 342.99, 357.82, 372.25, 386.30, 399.96, 413.25, 426.15]
C7H16 = [None, 27.81, 54.60, 80.52, 105.65, 130.08, 153.86, 177.02, 199.60, 221.62, 243.11, 264.07, 284.53, 304.48, 323.95, 342.95, 361.46, 379.51, 397.10, 414.24, 430.92, 447.15, 462.93, 478.28, 493.18]
C8H18 = [None, 31.65, 62.13, 91.60, 120.18, 147.95, 174.98, 201.31, 226.97, 251.99, 276.40, 300.21, 323.44, 346.11, 368.21, 389.77, 410.80, 431.28, 451.25, 470.69, 489.61, 508.02, 525.93, 543.32, 560.22]
# Plotting
plt.figure(figsize=(14, 8))
```

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```
plt.plot(temperature, CH4, marker='o', linestyle='-', color='red', label='Methane', markersize=10)
plt.plot(temperature, C2H6, marker='^', linestyle='-', color='blue', label='Ethane', markersize=10)
plt.plot(temperature, C3H8, marker='h', linestyle='-', color='green', label='Propane', markersize=10)
plt.plot(temperature, C4H10, marker='d', linestyle='-', color='purple', label='nButane', markersize=10)
plt.plot(temperature, C5H12, marker='X', linestyle='-', color='orange', label='nPentane', markersize=10)
plt.plot(temperature, C6H14, marker='p', linestyle='-', color='brown', label='nHexane', markersize=10)
plt.plot(temperature, C7H16, marker='v', linestyle='-', color='magenta', label='nHeptane', markersize=10)
plt.plot(temperature, C8H18, marker='*', linestyle='-', color='olive', label='nOctane', markersize=10)
# Adding titles and labels
plt.xlabel('Temperature (K)', fontsize=20)
plt.ylabel('Entropy Change ΔS (J/K)', fontsize=20)
plt.xticks(fontsize=14)  # Increase font size for x axis tick marks
plt.yticks(fontsize=14)  # Increase font size for y axis tick marks
plt.legend( fontsize=16)
plt.show()
```

2.3 Enthalpy of Formation (ΔH) Calculations:

To calculate enthalpy of formation at different temperatures the equation used from Kirchhoff's Law:

$$\Delta H_2 = \Delta H_1 + \int_{T_1}^{T_2} C_P dT \dots\dots\dots\dots\dots (9)$$

Where ΔH_1 is standard enthalpy of formation for the alkane at 298.15 K. On rewriting the equation (9)

$$\Delta H_2 = \Delta H_{f298} + \int_{298}^{T_2} C_P dT \dots\dots\dots (10)$$

For Methane $\Delta H_f^o{}_{298}$ =-74520 J/mol (Table 1) and $C_p = 14.15 + 75.499 \times 10^{-3}T - 17.99 \times 10^{-6}T^2$ (Equation 4):

$$\Delta H_2 = -74520 + \int_{298}^{T_2} (14.15 + 75.499 \times 10^{-3}T - 17.99 \times 10^{-6}T^2) dT \dots\dots\dots\dots\dots (11)$$

The values for ΔH_1, standard enthalpy of formation for the eight alkanes at 298.15 K is given in table 1. Herein, we have developed a python code that calculates and plots the enthalpy of formation over temperature range from 348 to 1498 for eight alkanes n-C_xH_{2x+2} (x=1 to 8).

2.3.1 Python Code for Enthalpy Chenge (ΔH) Calculation and Graph ΔH Vs T

```
import numpy as np
import matplotlib.pyplot as plt
# Constants
R = 8.314
a = 1.702
b = 9.081 * 10**-3
c = -2.164 * 10**-6
delH1 = -74520

# Temperature range
T_values = np.arange(298, 1499, 50)
delta_T = T_values[1] - T_values[0]

# Calculate Cp for each temperature
Cp_values = R * a + R * b * T_values + R * c * T_values**2

# Calculate integral of Cp_values
delH2_values = [delH1]
for i in range(1, len(T_values)):
    integral_Cp = np.trapz(Cp_values[:i+1], dx=delta_T)  # Numerical integration
    delH2 = delH1 + integral_Cp
    delH2_values.append(delH2)
```

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```
# Plot the graph with marker style 'd' and different color styles
plt.plot(T_values, delH2_values, marker='d', markerfacecolor="hotpink", linestyle='', markeredgewidth=1.5, color='hotpink', mec="b", ms=8)
plt.xlabel('Temperature (K)')
plt.ylabel('ΔH2 = ΔH1 + ∫Cp dT')
plt.title('Graph of ΔH')
plt.legend(['ΔH2 = ΔH1 + ∫Cp dT'], loc='upper left')
plt.grid(True)
plt.show()
# Printing table
print("Temperature (K)\t ΔH2")
for T, delH2 in zip(T_values, delH2_values):
    print(f"{T}\t\t {delH2}")
```

This program's output includes the enthalpy of formation (ΔH) values for methane gas across a temperature spectrum from 298 to 1498 K along with a plot for ΔH versus T. Using the same code ΔH for other alkanes can be computed and their corresponding graphs generated by merely changing standard enthalpy of formation [18,19] ΔH_1 at 298.15 K ($\Delta H_f^o{}_{298}$) from table 1 and variables A, B & C for each alkane.

Table 4: Values of Enthalpy change, ΔH ($J\ mol^{-1}$) for Methane, Ethane, *n*-Propane, *n*-Butane, *n*-Pentane, *n*-Hexane, *n*-Heptane and *n*-Octane

S. No.	T (K)	Enthalpy change (ΔH_2) ($Jmol^{-1}$)							
		CH_4	C_2H_6	*n*-C_3H_8	*n*-C_4H_{10}	*n*-C_5H_{12}	*n*-C_6H_{14}	*n*-C_7H_{16}	*n*-C_8H_{18}
1	298	-74520	-83820	-104680	-125790	-146760	-166920	-187780	-208750
2	348	-72688	-81011	-100696	-120526	-140262	-159182	-178804	-198536
3	398	-70698	-77883	-96241	-114661	-133026	-150570	-168819	-187176
4	448	-68555	-74447	-91334	-108216	-125080	-141119	-157865	-174717
5	498	-66264	-70716	-85992	-101217	-116455	-130864	-145983	-161204
6	548	-63828	-66700	-80236	-93686	-107179	-119841	-133212	-146684
7	598	-61254	-62411	-74082	-85648	-97282	-108083	-119594	-131204
8	648	-58544	-57860	-67549	-77126	-86793	-95626	-105170	-114808
9	698	-55704	-53060	-60655	-68144	-75741	-82505	-89978	-97544
10	748	-52738	-48022	-53419	-58725	-64157	-68754	-74061	-79457
11	798	-49651	-42757	-45859	-48894	-52068	-54409	-57459	-60594
12	848	-46446	-37276	-37994	-38673	-39505	-39504	-40212	-41000
13	898	-43129	-31593	-29841	-28087	-26497	-24075	-22360	-20722
14	948	-39704	-25717	-21420	-17160	-13073	-8155	-3944	194
15	998	-36176	-19661	-12748	-5915	738	8219	14995	21701
16	1048	-32549	-13436	-3843	5625	14905	25013	34417	43755
17	1098	-28827	-7053	5275	17435	29401	42192	54281	66308
18	1148	-25015	-525	14588	29492	44195	59722	74547	89314
19	1198	-21118	6137	24079	41772	59259	77567	95175	112728
20	1248	-17140	12922	33729	54252	74562	95692	116124	136503
21	1298	-13085	19819	43519	66907	90076	114063	137353	160593
22	1348	-8958	26814	53432	79714	105771	132644	158821	184951
23	1398	-4764	33898	63448	92650	121618	151401	180490	209533
24	1448	-507	41058	73550	105690	137587	170299	202317	234291
25	1498	3809	48283	83719	118812	153650	189303	224262	259179

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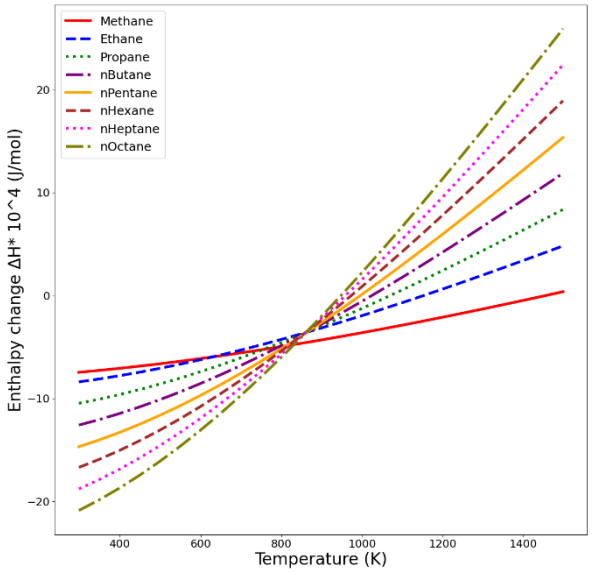

Figure 3: Enthalpy of Formation, ΔH Vs Temperature

The ΔH values for all eight alkanes, computed using Python code **2.3.1** are presented in table 4. While the output graphs of ΔH Vs temperature generated by this code are not displayed here, we developed another script **2.3.2** to plot combined graph of ΔH Vs temperature (Figure 3) for all alkanes. The data in table 4 demonstrates that enthalpy of formation (ΔH) increases across all alkanes as temperature rises from 298 K to 1498 K. This observed increase in ΔH correlates with the rise in C_p (as discussed in section **2.1**) with increasing temperature. Notably, this trend is more pronounced in higher alkanes compared to lower alkanes in the same temperature range.

2.3.2 Python Code to Plot ΔH Vs T for Eight Alkanes

```
import matplotlib.pyplot as plt
# Data
temperatures = [298, 348, 398, 448, 498, 548, 598, 648, 698, 748,
    798, 848, 898, 948, 998, 1048, 1098, 1148, 1198,
    1248, 1298, 1348, 1398, 1448, 1498]
enthalpy_change = {
"Methane": [-7.4520, -7.2688, -7.0698, -6.8555, -6.6264, -6.3828, -6.1254, -5.8544, -5.5704, -5.2738, -4.9651, -4.6446,
-4.3129, -3.9704, -3.6176, -3.2549, -2.8827, -2.5015, -2.1118, -1.7140, -1.3085, -0.8958, -0.4764, -0.0507, 0.3809],
    "Ethane": [-8.3820, -8.1011, -7.7883, -7.4447, -7.0716, -6.6700, -6.2411, -5.7860, -5.3060, -4.8022, -4.2757, -3.7276,
-3.1593, -2.5717, -1.9661, -1.3436, -0.7053, -0.0525, 0.6137, 1.2922, 1.9819, 2.6814, 3.3898, 4.1058, 4.8283],
    "Propane": [-10.4680, -10.0696, -9.6241, -9.1334, -8.5992, -8.0236, -7.4082, -6.7549, -6.0655, -5.3419, -4.5859, -
3.7994, -2.9841, -2.1420, -1.2748, -0.3843, 0.5275, 1.4588, 2.4079, 3.3729, 4.3519, 5.3432, 6.3448, 7.3550, 8.3719],
    "nButane": [-12.5790, -12.0526, -11.4661, -10.8216, -10.1217, -9.3686, -8.5648, -7.7126, -6.8144, -5.8725, -4.8894, -
3.8673, -2.8087, -1.7160, -0.5915, 0.5625, 1.7435, 2.9492, 4.1772, 5.4252, 6.6907, 7.9714, 9.2650, 10.5690, 11.8812],
    "nPentane": [-14.6760, -14.0262, -13.3026, -12.5080, -11.6455, -10.7179, -9.7282, -8.6793, -7.5741, -6.4157, -5.2068,
-3.9505, -2.6497, -1.3073, 0.0738, 1.4905, 2.9401, 4.4195, 5.9259, 7.4562, 9.0076, 10.5771, 12.1618, 13.7587, 15.3650],
    "nHexane": [-16.6920, -15.9182, -15.0570, -14.1119, -13.0864, -11.9841, -10.8083, -9.5626, -8.2505, -6.8754, -
5.4409, -3.9504, -2.4075, -0.8155, 0.8219, 2.5013, 4.2192, 5.9722, 7.7567, 9.5692, 11.4063, 13.2644, 15.1401, 17.0299,
18.9303],
    "nHeptane": [-18.7780, -17.8804, -16.8819, -15.7865, -14.5983, -13.3212, -11.9594, -10.5170, -8.9978, -7.4061, -
5.7459, -4.0212, -2.2360, -0.3944, 1.4995, 3.4417, 5.4281, 7.4547, 9.5175, 11.6124, 13.7353, 15.8821, 18.0490, 20.2317,
22.4262],
    "nOctane": [-20.8750, -19.8536, -18.7176, -17.4717, -16.1204, -14.6684, -13.1204, -11.4808, -9.7544, -7.9457, -
6.0594, -4.1000, -2.0722, 0.0194, 2.1701, 4.3755, 6.6308, 8.9314, 11.2728, 13.6503, 16.0593, 18.4951, 20.9533, 23.4291,
25.9179]
}# Plotting
plt.figure(figsize=(14, 12))
# Define line styles and colors for each gas
```

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```
styles = {  "Methane": ("-", "red"),
    "Ethane": ("--", "blue"),
    "Propane": (":", "green"),
    "nButane": ("-.", "purple"),
    "nPentane": ("-", "orange"),
    "nHexane": ("--", "brown"),
    "nHeptane": (":", "magenta"),
    "nOctane": ("-.", "olive")}
# Plot each gas with the corresponding style and color
for gas, (style, color) in styles.items():
    plt.plot(temperatures, enthalpy_change[gas], linestyle=style, linewidth=4, color=color, label=gas)
# Adding labels and title
plt.xlabel('Temperature (K)', fontsize=24)
plt.ylabel('Enthalpy change ΔH* 10^4 (J/mol)', fontsize=24)
plt.xticks(fontsize=16)  # Increase font size for x axis tick marks
plt.yticks(fontsize=16)  # Increase font size for y axis tick marks
plt.legend(fontsize=18)
plt.show()
```

2.4 Gibb's Free energy (ΔG) Calculations:

Gibb's Free energy, ΔG for any system can be determined using following equation:

$$\Delta G = \Delta H_2 - T\Delta S \ldots\ldots\ldots (12)$$

Here, ΔH_2 represents enthalpy of formation calculated at various temperatures discussed in section 2.3, while ΔS denotes the entropy change at different temperatures calculated in section 2.2. Here we have developed python code to compute ΔG for eight alkanes n-C_xH_{2x+2} (x=1 to 8) over the temperature range 298 to 1498 kelvin using the equation (12).

2.4.1 Python Code for Gibb's Free energy (ΔG) Calculation and Graph ΔG Vs T

```
import numpy as np
import matplotlib.pyplot as plt
# Constants for delH2 calculation
R = 8.314
a = 1.702
b = 9.081 * 10**-3
c = -2.164 * 10**-6
delH1 = -74520
# Constants for delS calculation
A = 14.150428  # This is the value of R *a thats why we can also write as
A1 = R * a
B = 0.075499434
B1 = R * b
C = -0.000017991496
C1 = R * b
# Temperature range with interval T_values = np.arange(298, 1499, 50)
# Calculate Cp for each temperature Cp_values = R * a + R * b * T_values + R * c * T_values**2
# Calculate delH2 for each temperature delta_T = T_values[1] - T_values[0]
delH2_values = [delH1]
for i in range(1, len(T_values)):
    # Calculate integral of Cp_values using trapezoidal rule
    integral_Cp = np.trapz(Cp_values[:i+1], T_values[:i+1])
    delH2 = delH1 + integral_Cp
    delH2_values.append(delH2)
# Calculate delS for each temperature
T_min = T_values[0]
delS_values = []
for T in T_values:
    delS_A = A * (np.log(T) - np.log(T_min))
    delS_B = B * (T - T_min)
```

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```
    delS_C = 0.5 * C * (T**2 - T_min**2)
    delS = delS_A + delS_B + delS_C
    delS_values.append(delS)

# Calculate delG for each temperature
delG_values = []
for T, delH2, delS in zip(T_values, delH2_values, delS_values):
    delG = delH2 - T * delS
    delG_values.append(delG)

plt.figure(figsize=(8, 6))  # Adjust the size of Graph for a clear view
# Plot the graph for delG vs T
plt.plot(T_values, delG_values, color='Red', label='Methane', marker='*', markersize=10, linestyle='-')
plt.xlabel('Temperature (K)')
plt.ylabel('ΔG(J/mol)')

plt.legend(loc='upper right')
plt.grid(True)
plt.show()

# Printing table for delG values
print("Temperature (K)\t delG")
for T, delG in zip(T_values, delG_values):
    print(f"{T}\t\t {delG}")
```

This program calculates Gibb's Free energy (ΔG) values for methane gas across the temperature range 298 to 1498 K and generates a plot for ΔG vs T. The same code can easily be adapted to calculate ΔG for other alkanes by changing the variables A, B, C and ΔH_1 (Table 1) specific to each alkane.

Table 5: Values of Gibb's Free energy, ΔG ($J\ mol^{-1}$) for Methane, Ethane, *n*-Propane, *n*-Butane, *n*-Pentane, *n*-Hexane, *n*-Heptane and *n*-Octane

S. No.	T (K)	Gibb's Free Energy, ΔG ($Jmol^{-1}$)							
		CH_4	C_2H_6	*n*-C_3H_8	*n*-C_4H_{10}	*n*-C_5H_{12}	*n*-C_6H_{14}	*n*-C_7H_{16}	*n*-C_8H_{18}
1	298	-	-	-	-	-	-	-	-
2	348	-74663	-84039	-104986	-126202	-147269	-167515	-188474	-209541
3	398	-75083	-84687	-105898	-127415	-148766	-169283	-190530	-211883
4	448	-75762	-85747	-107397	-129402	-151218	-172185	-193901	-215721
5	498	-76688	-87207	-109467	-132141	-154596	-176183	-198544	-221009
6	548	-77853	-89057	-112092	-135609	-158874	-181248	-204424	-227704
7	598	-79246	-91285	-115261	-139789	-164027	-187350	-211506	-235767
8	648	-80860	-93884	-118958	-144661	-170033	-194462	-219759	-245164
9	698	-82688	-96844	-123172	-150209	-176871	-202558	-229153	-255859
10	748	-84724	-100156	-127891	-156417	-184520	-211615	-239660	-267821
11	798	-86963	-103813	-133103	-163269	-192960	-221607	-251251	-281019
12	848	-89399	-107807	-138798	-170749	-192960	-232514	-263901	-295422
13	898	-92028	-112130	-144963	-178843	-212142	-244312	-277584	-311001
14	948	-94844	-116775	-151588	-187536	-222846	-256980	-292274	-327729
15	998	-97844	-121735	-158663	-196814	-234269	-270497	-307948	-345576
16	1048	-101023	-127002	-166176	-206664	-246393	-284842	-324580	-364516
17	1098	-104377	-132571	-174118	-217070	-259201	-299994	-342148	-384522
18	1148	-107903	-138433	-182479	-228021	-272677	-315935	-360627	-405566
19	1198	-111597	-144584	-191247	-239501	-286803	-332642	-379995	-427624
20	1248	-115455	-151014	-200414	-251499	-301563	-350098	-400228	-450668
21	1298	-119474	-157719	-209969	-264000	-316941	-368281	-421304	-474674
22	1348	-123651	-164692	-219902	-276992	-332920	-387174	-443200	-499615
23	1398	-127982	-171926	-230203	-290462	-349484	-406756	-465894	-525467

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24	1448	-132465	-179414	-240862	-304396	-366618	-427009	-489363	-552203
25	1498	-137095	-187152	-251870	-318782	-384304	-447913	-513587	-579801

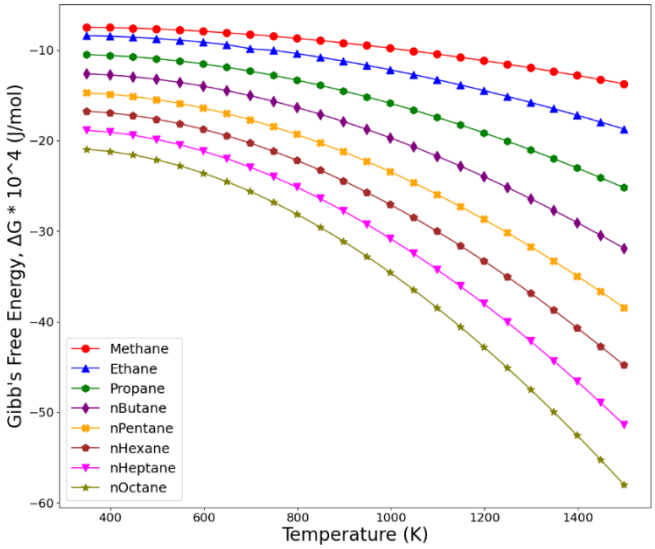

Figure 4: Gibb's Free energy, ΔG Vs Temperature

The ΔG values for all eight alkanes, computed using Python code **2.4.1** are presented in table 5. Although the individual graphs of ΔG Vs temperature generated by this code are not shown here, we have written a supplementary script **2.4.2** to plot a combined graph of ΔG Vs temperature for all alkanes, like C_p Vs temperature. The combined graph is depicted in Figure 4. The data in table 5 demonstrates that Gibb's Free energy (ΔG) decreases for all alkanes as temperature rises from 298 K to 1498 K. This observed decrease in ΔG indicates greater spontaneity of alkane with rising temperature. Notably, this trend is more pronounced in higher alkanes compared to lower alkanes within the same temperature range.

2.4.2 Python Code to Plot ΔG Vs T for Eight Alkanes

```
import matplotlib.pyplot as plt
# Data
temperature = [298, 348, 398, 448, 498, 548, 598, 648, 698, 748, 798, 848, 898, 948, 998, 1048, 1098, 1148, 1198, 1248, 1298, 1348, 1398, 1448, 1498]
CH4 = [None, -7.4663, -7.5083, -7.5762, -7.6688, -7.7853, -7.9246, -8.0860, -8.2688, -8.4724, -8.6963, -8.9399, -9.2028, -9.4844, -9.7844, -10.1023, -10.4377, -10.7903, -11.1597, -11.5455, -11.9474, -12.3651, -12.7982, -13.2465, -13.7095]
C2H6 = [None, -8.4039, -8.4687, -8.5747, -8.7207, -8.9057, -9.1285, -9.3884, -9.844, -10.0156, -10.3813, -10.7807, -11.2130, -11.6775, -12.1735, -12.7002, -13.2571, -13.8433, -14.4584, -15.1014, -15.7719, -16.4692, -17.1926, -17.9414, -18.7152]
C3H8 = [None, -10.4986, -10.5898, -10.7397, -10.9467, -11.2092, -11.5261, -11.8958, -12.3172, -12.7891, -13.3103, -13.8798, -14.4963, -15.1588, -15.8663, -16.6176, -17.4118, -18.2479, -19.1247, -20.0414, -20.9969, -21.9902, -23.0203, -24.0862, -25.1870]
C4H10 = [None, -12.6202, -12.7415, -12.9402, -13.2141, -13.5609, -13.9789, -14.4661, -15.0209, -15.6417, -16.3269, -17.0749, -17.8843, -18.7536, -19.6814, -20.6664, -21.7070, -22.8021, -23.9501, -25.1499, -26.4000, -27.6992, -29.0462, -30.4396, -31.8782]
C5H12 = [None, -14.7269, -14.8766, -15.1218, -15.4596, -15.8874, -16.4027, -17.0033, -17.6871, -18.4520, -19.2960, -20.2558, -21.2142, -22.2846, -23.4269, -24.6393, -25.9201, -27.2677, -28.6803, -30.1563, -31.6941, -33.2920, -34.9484, -36.6618, -38.4304]
C6H14 = [None, -16.7515, -16.9283, -17.2185, -17.6183, -18.1248, -18.7350, -19.4462, -20.2558, -21.1615, -22.1607, -23.2514, -24.4312, -25.6980, -27.0497, -28.4842, -29.9994, -31.5935, -33.2642, -35.0098, -36.8281, -38.7174, -40.6756, -42.7009, -44.7913]
C7H16 = [None, -18.8474, -19.0530, -19.3901, -19.8544, -20.4424, -21.1506, -21.9759, -22.9153, -23.9660, -25.1251, -26.3901, -27.7584, -29.2274, -30.7948, -32.4580, -34.2148, -36.0627, -37.9995, -40.0228, -42.1304, -44.3200, -46.5894, -48.9363, -51.3587]
```

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```
C8H18 = [None, -20.9541, -21.1883, -21.5721, -22.1009, -22.7704, -23.5767, -24.5164, -25.5859, -26.7821, -28.1019, -29.5422, -31.1001, -32.7729, -34.5576, -36.4516, -38.4522, -40.5566, -42.7624, -45.0668, -47.4674, -49.9615, -52.5467, -55.2203, -57.9801]
# Plotting
plt.figure(figsize=(14, 12))
plt.plot(temperature, CH4, marker='o', linestyle='-', color='red', label='Methane', markersize=10)
plt.plot(temperature, C2H6, marker='^', linestyle='-', color='blue', label='Ethane', markersize=10)
plt.plot(temperature, C3H8, marker='h', linestyle='-', color='green', label='Propane', markersize=10)
plt.plot(temperature, C4H10, marker='d', linestyle='-', color='purple', label='nButane', markersize=10)
plt.plot(temperature, C5H12, marker='X', linestyle='-', color='orange', label='nPentane', markersize=10)
plt.plot(temperature, C6H14, marker='p', linestyle='-', color='brown', label='nHexane', markersize=10)
plt.plot(temperature, C7H16, marker='v', linestyle='-', color='magenta', label='nHeptane', markersize=10)
plt.plot(temperature, C8H18, marker='*', linestyle='-', color='olive', label='nOctane', markersize=10)
plt.xlabel('Temperature (K)', fontsize=24)
plt.ylabel("Gibb's Free Energy, ΔG * 10^4 (J/mol)", fontsize=24)
plt.xticks(fontsize=16)  # Increase font size for x axis tick marks
plt.yticks(fontsize=16)  # Increase font size for y axis tick marks
plt.legend( fontsize=18)
plt.show()
```

3. Conclusions

The present work emphasizes the crucial role of lower alkanes in fuel applications and highlights the significance of comprehending their thermodynamic properties. Through Python-based calculations, we successfully computed four pivotal thermodynamic parameters: C_p, ΔS, ΔH and ΔG for eight alkanes across a broad temperature spectrum. This approach sheds light on heat capacity, enthalpy, entropy, and Gibbs free energy changes, offering insights into reaction spontaneity and energy dynamics. The developed Python code in the present article enables the creation of a comprehensive library of thermodynamic data. Python's efficiency and flexibility proved instrumental in streamlining these calculations, enhancing accessibility, and facilitating deeper analysis. Our work not only contributes to advance scientific understanding but also underscores the growing importance of computational tools like python in tackling complex thermodynamic challenges.

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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interests.

CONTRIBUTION OF AUTHORS

All the authors contributed significantly to the manuscript, participating in writing/ reviewing/ editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCHID ids, given below:

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