

Supporting Information

A Combined Experimental and Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates I: *n*-Decane (*n*-C₁₀H₂₂)

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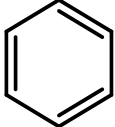
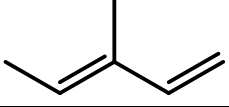
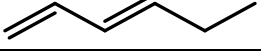
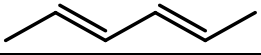
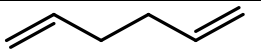
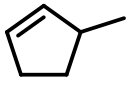
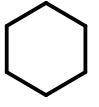
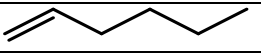
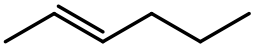
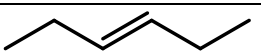
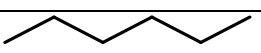
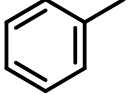
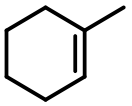
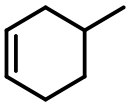
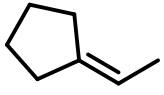
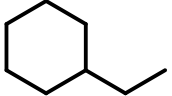
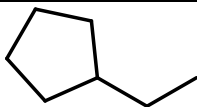
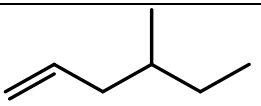
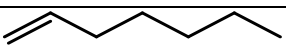
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Table S1. Molecules detected in previous pyrolysis studies of *n*-decane.

Molecule	Formula	Mass	Structure	Ref.
Hydrogen	H ₂	2	H—H	1-3
Methyl	CH ₃	15	CH ₃ •	1,3
Methane	CH ₄	16	CH ₄	1-5
Acetylene	C ₂ H ₂	26		1,3-5
Ethylene	C ₂ H ₄	28		1-5
Ethane	C ₂ H ₆	30		2,4-5
Propargyl	C ₃ H ₃	39		1,3
Allene	C ₃ H ₄	40		1,3,5
Methylacetylene	C ₃ H ₄	40		1,3,5
Allyl	C ₃ H ₅	41		1,3
Propene	C ₃ H ₆	42		1-5
Propane	C ₃ H ₈	44		2
Diacetylene	C ₄ H ₂	50		5
Vinylacetylene	C ₄ H ₄	52		5
1,3-Butadiene	C ₄ H ₆	54		1,3-5
1-Butene	C ₄ H ₈	56		1-6
2-Butene	C ₄ H ₈	56		1,3
<i>n</i> -Butane	C ₄ H ₁₀	58		2
1,3-Pentadiene	C ₅ H ₈	68		1,3
1,4-Pentadiene	C ₅ H ₈	68		6
Cyclopentene	C ₅ H ₈	68		6
1-Pentene	C ₅ H ₁₀	70		1-6
Cyclopentane	C ₅ H ₁₀	70		6
<i>trans</i> -2-Pentene	C ₅ H ₁₀	70		6
<i>cis</i> -2-Pentene	C ₅ H ₁₀	70		6
<i>n</i> -Pentane	C ₅ H ₁₂	72		2

Benzene	C_6H_6	78		1,3,5
3-Methyl-1,3-pentadiene	C_6H_8	80		6
1,3-Hexadiene	C_6H_{10}	82		1,3
2,4-Hexadiene	C_6H_{10}	82		6
1,5-Hexadiene	C_6H_{10}	82		5-6
3-Methyl-cyclopentene	C_6H_{10}	82		6
Cyclohexane	C_6H_{12}	84		6
1-Hexene	C_6H_{12}	84		1-6
2-Hexene	C_6H_{12}	84		6
3-Hexene	C_6H_{12}	84		6
<i>n</i> -Hexane	C_6H_{14}	86		2,6
Toluene	C_7H_8	92		5
1-Methyl-cyclohexene	C_7H_{12}	96		6
4-Methyl-cyclohexene	C_7H_{12}	96		6
Ethylidene-cyclopentane	C_7H_{12}	96		6
Ethyl-cyclohexane	C_7H_{14}	98		6
Ethyl-cyclopentane	C_7H_{14}	98		6
4-Methyl-1-hexene	C_7H_{14}	98		6
1-Heptene	C_7H_{14}	98		1-3,5-6

<i>trans</i> -2-Heptene	C ₇ H ₁₄	98		6
<i>cis</i> -2-Heptene	C ₇ H ₁₄	98		6
<i>n</i> -Heptane	C ₇ H ₁₆	100		2,6
1-Octene	C ₈ H ₁₆	112		1-3,5-6
<i>trans</i> -2-Octene	C ₈ H ₁₆	112		6
<i>cis</i> -2-Octene	C ₈ H ₁₆	112		6
Methyl-cycloheptane	C ₈ H ₁₆	112		6
<i>n</i> -Octane	C ₈ H ₁₈	114		2,6
1-Nonene	C ₉ H ₁₈	126		1-3,5-6
2-Nonene	C ₉ H ₁₈	126		6
1,1,3-Trimethyl-cyclohexane	C ₉ H ₁₈	126		6
1-Methyl-1-ethyl-cyclohexane	C ₉ H ₁₈	126		6
Propyl-cyclohexane	C ₉ H ₁₈	126		6
<i>n</i> -Nonane	C ₉ H ₂₀	128		2,6
Naphthalene	C ₁₀ H ₈	128		6
Octahydro-4,7-methano-1H-indene	C ₁₀ H ₁₆	136		6
<i>trans</i> -Decahydro-naphthalene	C ₁₀ H ₁₈	138		6
1-Decene	C ₁₀ H ₂₀	140		1,3,6
2-Decene	C ₁₀ H ₂₀	140		6
4-Decene	C ₁₀ H ₂₀	140		6

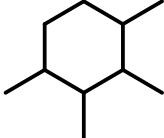
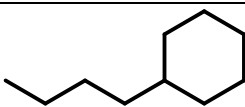
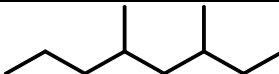
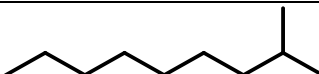
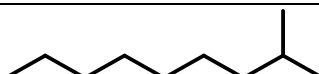
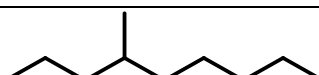
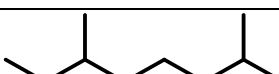
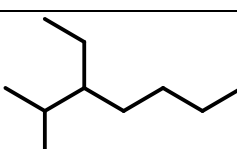




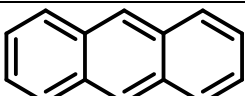
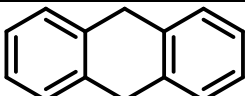
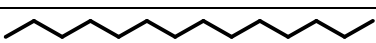



1,2,3,4-Tetramethyl-cyclohexane	$C_{10}H_{20}$	140		6
Butyl-cyclohexane	$C_{10}H_{20}$	140		6
3,5-Dimethyl-octane	$C_{10}H_{22}$	142		6
2-Methyl-nonane	$C_{10}H_{22}$	142		6
3-Methyl-nonane	$C_{10}H_{22}$	142		6
4-Methyl-nonane	$C_{10}H_{22}$	142		6
2,6-Dimethyl-octane	$C_{10}H_{22}$	142		6
3-Ethyl-2-methyl-heptan	$C_{10}H_{22}$	142		6
<i>n</i> -decane	$C_{10}H_{22}$	142		1-6
<i>n</i> -Undecane	$C_{11}H_{24}$	156		6
<i>n</i> -Dodecane	$C_{12}H_{26}$	170		6
<i>n</i> -Tridecane	$C_{13}H_{28}$	184		6
Anthracene	$C_{14}H_{10}$	178		6
9,10-Dihydro-anthracene	$C_{14}H_{12}$	180		6
<i>n</i> -Tetradecane	$C_{14}H_{30}$	198		6
<i>n</i> -Hexadecane	$C_{16}H_{34}$	226		6
<i>n</i> -Heptadecane	$C_{17}H_{36}$	228		6
<i>n</i> -Eicosane	$C_{20}H_{42}$	282		6

Table S2. Mole fractions of the products observed in the decomposition of *n*-decane at 600 Torr in the chemical reactor at 1100, 1200, 1300, 1400, 1500 and 1600 K.

Species*	Formula	Mass	Temperature					
			1100 K	1200 K	1300 K	1400 K	1500 K	1600 K
Hydrogen	H ₂	2	0.00E+00	1.11E-06	4.30E-06	9.94E-06	2.14E-05	1.76E-04
Methyl radical	CH ₃	15	0.00E+00	1.46E-05	1.33E-04	2.95E-04	2.59E-04	3.78E-06
Methane	CH ₄	16	0.00E+00	0.00E+00	4.86E-07	1.30E-06	1.85E-06	1.29E-06
Acetylene	C ₂ H ₂	26	5.78E-07	0.00E+00	5.45E-07	2.96E-06	1.00E-05	2.55E-05
Vinyl radical	C ₂ H ₃	27	4.89E-07	4.87E-07	4.71E-07	1.27E-06	1.12E-06	0.00E+00
Ethylene	C ₂ H ₄	28	5.54E-06	4.53E-05	3.96E-04	1.01E-03	1.03E-03	5.06E-04
Ethyl radical	C ₂ H ₅	29	0.00E+00	1.57E-05	5.02E-05	1.70E-05	2.81E-06	1.88E-06
Propargyl radical	C ₃ H ₃	39	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.04E-06	2.57E-07
Allene	C ₃ H ₄	40	0.00E+00	0.00E+00	5.95E-07	1.39E-05	4.65E-05	1.31E-05
Methylacetylene	C ₃ H ₄	40	0.00E+00	0.00E+00	4.62E-07	1.07E-05	4.01E-05	1.32E-05
Allyl radical	C ₃ H ₅	41	6.76E-07	9.20E-07	1.40E-05	7.16E-05	3.60E-05	8.79E-07
Propene	C ₃ H ₆	42	2.82E-06	1.33E-05	8.89E-05	1.69E-04	1.53E-04	5.61E-05
1,3-Butadiene	C ₄ H ₆	54	0.00E+00	0.00E+00	1.02E-06	4.42E-06	5.11E-06	9.82E-07
1-Butene	C ₄ H ₈	56	4.60E-06	9.11E-06	3.50E-05	3.27E-05	5.52E-06	2.52E-07
2-Butene	C ₄ H ₈	56	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.09E-06	4.39E-08
1-Pentene	C ₅ H ₁₀	70	0.00E+00	2.62E-06	1.21E-05	6.51E-06	4.42E-07	0.00E+00
1-Hexene	C ₆ H ₁₂	84	0.00E+00	1.33E-06	1.36E-05	4.46E-06	0.00E+00	0.00E+00
<i>n</i> -Decane	C ₁₀ H ₂₂	142	1.99E-04	1.92E-04	1.27E-04	7.33E-06	6.24E-07	0.00E+00

Table S3. Product branching ratios for dissociation of C₅H₁₁ (1-pentyl radical) calculated at various temperatures and pressures within RRHO approximation.

T(K)	30 Torr			1 atm			10 atm			100 atm		
	C ₃ H ₇ + C ₂ H ₄	C ₂ H ₅ + C ₃ H ₆	C ₅ H ₁₀ + H	C ₃ H ₇ + C ₂ H ₄	C ₂ H ₅ + C ₃ H ₆	C ₅ H ₁₀ + H	C ₃ H ₇ + C ₂ H ₄	C ₂ H ₅ + C ₃ H ₆	C ₅ H ₁₀ + H	C ₃ H ₇ + C ₂ H ₄	C ₂ H ₅ + C ₃ H ₆	C ₅ H ₁₀ + H
500	38.85%	61.13%	0.02%	91.47%	8.44%	0.09%	98.93%	0.97%	0.10%	99.80%	0.10%	0.10%
600	31.28%	68.69%	0.03%	84.08%	15.74%	0.19%	97.53%	2.23%	0.24%	99.51%	0.24%	0.25%
700	27.09%	72.86%	0.05%	75.39%	24.33%	0.29%	94.86%	4.69%	0.44%	98.96%	0.55%	0.49%
800	25.46%	74.48%	0.06%	68.06%	31.57%	0.37%	90.98%	8.35%	0.67%	98.02%	1.19%	0.79%
900	25.62%	74.30%	0.07%	63.59%	35.97%	0.45%	86.78%	12.34%	0.88%	96.61%	2.25%	1.13%
1000	26.81%	73.10%	0.09%	61.80%	37.67%	0.52%	83.41%	15.53%	1.06%	94.83%	3.68%	1.49%
1100	28.49%	71.40%	0.11%	61.75%	37.65%	0.60%	81.36%	17.40%	1.23%	92.99%	5.18%	1.83%
1200	30.38%	69.48%	0.14%	62.57%	36.74%	0.69%	80.44%	18.16%	1.40%	91.41%	6.44%	2.14%
1300	32.36%	67.47%	0.17%	63.78%	35.44%	0.78%	80.24%	18.20%	1.56%	90.26%	7.31%	2.44%
1400	34.36%	65.45%	0.19%	65.13%	34.00%	0.87%	80.44%	17.85%	1.72%	89.50%	7.79%	2.71%
1500	36.34%	63.44%	0.23%	66.49%	32.56%	0.95%	80.82%	17.31%	1.87%	89.04%	8.00%	2.97%
1600	38.27%	61.47%	0.26%	67.80%	31.16%	1.04%	81.29%	16.69%	2.02%	88.78%	8.02%	3.21%
1700	40.17%	59.53%	0.29%	69.04%	29.83%	1.13%	81.78%	16.06%	2.16%	88.64%	7.92%	3.44%
1800	42.00%	57.66%	0.33%	70.21%	28.58%	1.22%	82.27%	15.43%	2.30%	88.58%	7.77%	3.65%
1900	43.76%	55.86%	0.37%	71.29%	27.41%	1.30%	82.73%	14.84%	2.43%	88.56%	7.58%	3.86%
2000	45.45%	54.14%	0.42%	72.29%	26.32%	1.39%	83.17%	14.27%	2.56%	88.57%	7.37%	4.06%
2100	47.10%	52.43%	0.47%	73.24%	25.29%	1.48%	83.58%	13.74%	2.69%	88.59%	7.16%	4.24%
2200	48.52%	50.97%	0.51%	74.09%	24.34%	1.56%	83.95%	13.24%	2.81%	88.62%	6.96%	4.43%
2300	49.83%	49.61%	0.57%	74.89%	23.46%	1.65%	84.30%	12.77%	2.93%	88.65%	6.75%	4.60%
2400	50.80%	48.58%	0.62%	75.63%	22.63%	1.74%	84.62%	12.33%	3.05%	88.67%	6.56%	4.77%
2500	51.56%	47.77%	0.67%	76.34%	21.83%	1.82%	84.92%	11.91%	3.17%	88.70%	6.37%	4.93%

Table S4. Product branching ratios for dissociation of C₆H₁₃ (1-hexyl radical) calculated at various temperatures and pressures within RRHO approximation.

T(K)	30 Torr					1 atm				
	C ₄ H ₉ + C ₂ H ₄	C ₃ H ₇ + C ₃ H ₆	C ₂ H ₅ + C ₄ H ₈	CH ₃ + C ₅ H ₁₀	C ₆ H ₁₂ + H	C ₄ H ₉ + C ₂ H ₄	C ₃ H ₇ + C ₃ H ₆	C ₂ H ₅ + C ₄ H ₈	CH ₃ + C ₅ H ₁₀	C ₆ H ₁₂ + H
500	6.57%	88.24%	3.84%	1.34%	0.01%	56.23%	41.71%	1.46%	0.54%	0.05%
600	6.79%	83.11%	7.26%	2.83%	0.01%	42.05%	54.01%	2.72%	1.13%	0.09%
700	7.13%	76.52%	11.56%	4.77%	0.02%	30.49%	63.03%	4.38%	1.97%	0.12%
800	7.13%	67.96%	17.42%	7.46%	0.03%	23.59%	67.07%	6.22%	2.97%	0.14%
900						20.24%	67.73%	7.92%	3.94%	0.17%
1000						18.77%	66.95%	9.30%	4.78%	0.20%
1100						18.08%	65.72%	10.45%	5.51%	0.23%
1200						17.67%	64.44%	11.45%	6.18%	0.26%
T(K)	10 atm					100 atm				
	C ₄ H ₉ + C ₂ H ₄	C ₃ H ₇ + C ₃ H ₆	C ₂ H ₅ + C ₄ H ₈	CH ₃ + C ₅ H ₁₀	C ₆ H ₁₂ + H	C ₄ H ₉ + C ₂ H ₄	C ₃ H ₇ + C ₃ H ₆	C ₂ H ₅ + C ₄ H ₈	CH ₃ + C ₅ H ₁₀	C ₆ H ₁₂ + H
500	92.54%	6.99%	0.26%	0.10%	0.11%	99.09%	0.75%	0.03%	0.01%	0.12%
600	86.61%	12.17%	0.68%	0.29%	0.25%	98.18%	1.41%	0.08%	0.03%	0.29%
700	77.44%	19.92%	1.52%	0.72%	0.41%	96.49%	2.63%	0.21%	0.10%	0.56%
800	66.63%	28.58%	2.82%	1.42%	0.55%	93.74%	4.62%	0.50%	0.26%	0.88%
900	57.09%	35.66%	4.31%	2.29%	0.66%	89.86%	7.34%	1.01%	0.56%	1.24%
1000	50.64%	39.88%	5.63%	3.10%	0.75%	85.31%	10.37%	1.73%	1.00%	1.59%
1100	47.27%	41.56%	6.58%	3.74%	0.85%	80.98%	13.08%	2.53%	1.51%	1.90%
1200	46.06%	41.60%	7.19%	4.19%	0.96%	77.64%	14.94%	3.23%	1.99%	2.20%
1300	46.15%	40.74%	7.54%	4.49%	1.09%	75.54%	15.88%	3.73%	2.37%	2.48%
1400	46.97%	39.42%	7.71%	4.68%	1.23%	74.50%	16.07%	4.05%	2.62%	2.76%
1500	48.18%	37.89%	7.77%	4.78%	1.37%	74.19%	15.78%	4.22%	2.78%	3.04%
1600	49.59%	36.29%	7.75%	4.84%	1.52%	74.33%	15.22%	4.28%	2.86%	3.32%
1700						74.71%	14.53%	4.27%	2.89%	3.59%
1800						75.22%	13.80%	4.22%	2.90%	3.86%

1900	75.78%	13.07%	4.15%	2.88%	4.12%
2000	76.35%	12.37%	4.06%	2.84%	4.37%
2100	76.90%	11.71%	3.97%	2.80%	4.62%

Table S5. Product branching ratios for dissociation of C₇H₁₅ (1-heptyl radical) calculated at various temperatures and pressures within RRHO approximation.

T(K)	30 Torr						1 atm					
	C ₅ H ₁₁ + C ₂ H ₄	C ₄ H ₉ + C ₃ H ₆	CH ₃ + C ₆ H ₁₂	C ₃ H ₇ + C ₄ H ₈	C ₂ H ₅ + C ₅ H ₁₀	C ₇ H ₁₄ + H	C ₅ H ₁₁ + C ₂ H ₄	C ₄ H ₉ + C ₃ H ₆	CH ₃ + C ₆ H ₁₂	C ₃ H ₇ + C ₄ H ₈	C ₂ H ₅ + C ₅ H ₁₀	C ₇ H ₁₄ + H
500	8.86%	23.88%	21.46%	42.80%	2.98%	0.00%	68.73%	5.25%	8.72%	16.22%	1.03%	0.05%
600	6.63%	32.35%	19.62%	35.84%	5.55%	0.01%	50.33%	9.24%	14.08%	24.04%	2.22%	0.09%
700	5.82%	38.19%	17.13%	29.34%	9.50%	0.02%	33.99%	14.37%	18.27%	29.34%	3.93%	0.10%
800	4.91%	38.87%	13.46%	21.86%	20.89%	0.02%	23.82%	19.32%	20.04%	30.73%	5.98%	0.11%
900							18.59%	22.89%	20.23%	29.96%	8.20%	0.12%
1000							15.66%	25.37%	19.72%	28.40%	10.72%	0.13%
1100							13.22%	27.59%	18.62%	26.23%	14.21%	0.13%
T(K)	10 atm						100 atm					
	C ₅ H ₁₁ + C ₂ H ₄	C ₄ H ₉ + C ₃ H ₆	CH ₃ + C ₆ H ₁₂	C ₃ H ₇ + C ₄ H ₈	C ₂ H ₅ + C ₅ H ₁₀	C ₇ H ₁₄ + H	C ₅ H ₁₁ + C ₂ H ₄	C ₄ H ₉ + C ₃ H ₆	CH ₃ + C ₆ H ₁₂	C ₃ H ₇ + C ₄ H ₈	C ₂ H ₅ + C ₅ H ₁₀	C ₇ H ₁₄ + H
500	95.46%	0.72%	1.26%	2.32%	0.16%	0.09%	99.44%	0.07%	0.13%	0.24%	0.02%	0.09%
600	90.13%	1.59%	2.85%	4.74%	0.48%	0.20%	98.69%	0.17%	0.32%	0.53%	0.06%	0.23%
700	80.90%	3.25%	5.59%	8.68%	1.25%	0.33%	97.18%	0.39%	0.72%	1.11%	0.17%	0.43%
800	69.00%	5.67%	9.02%	13.30%	2.57%	0.43%	94.54%	0.80%	1.45%	2.10%	0.43%	0.68%
900	57.85%	8.30%	12.02%	17.03%	4.29%	0.51%	90.60%	1.45%	2.54%	3.51%	0.95%	0.95%
1000	50.05%	10.37%	13.89%	19.08%	6.04%	0.56%	85.81%	2.28%	3.84%	5.12%	1.74%	1.21%
1100	45.76%	11.54%	14.74%	19.77%	7.56%	0.62%	81.15%	3.11%	5.04%	6.53%	2.71%	1.44%
1200	43.90%	11.97%	14.96%	19.67%	8.80%	0.69%	77.54%	3.75%	5.91%	7.48%	3.66%	1.66%
1300	43.47%	11.97%	14.81%	19.18%	9.79%	0.78%	75.29%	4.11%	6.37%	7.91%	4.45%	1.86%
1400	43.82%	11.74%	14.49%	18.51%	10.58%	0.86%	74.19%	4.24%	6.51%	7.96%	5.03%	2.07%
1500							73.88%	4.21%	6.45%	7.77%	5.42%	2.27%
1600							74.05%	4.08%	6.26%	7.46%	5.67%	2.48%
1700							74.48%	3.92%	6.02%	7.10%	5.80%	2.68%
1800							75.06%	3.73%	5.75%	6.73%	5.85%	2.88%
1900							75.97%	3.52%	5.41%	6.32%	5.75%	3.04%

2000

76.39% 3.37% 5.20% 6.01% 5.80% 3.23%

Table S6. Product branching ratios for dissociation of C₈H₁₇ (1-octyl radical) calculated at various temperatures and pressures within RRHO approximation.

T(K)	30 Torr							1 atm						
	C ₆ H ₁₃ + C ₂ H ₄	C ₅ H ₁₁ + C ₃ H ₆	CH ₃ + C ₇ H ₁₄	C ₄ H ₉ + C ₄ H ₈	C ₂ H ₅ + C ₆ H ₁₂	C ₃ H ₇ + C ₅ H ₁₀	C ₈ H ₁₆ + H	C ₆ H ₁₃ + C ₂ H ₄	C ₅ H ₁₁ + C ₃ H ₆	CH ₃ + C ₇ H ₁₄	C ₄ H ₉ + C ₄ H ₈	C ₂ H ₅ + C ₆ H ₁₂	C ₃ H ₇ + C ₅ H ₁₀	C ₈ H ₁₆ + H
500	4.76%	6.57%	2.16%	4.38%	50.38%	31.75%	0.00%	56.28%	0.92%	1.03%	1.98%	24.06%	15.65%	0.07%
600	3.13%	12.16%	3.95%	7.07%	44.43%	29.25%	0.01%	37.18%	2.43%	1.81%	3.09%	32.98%	22.40%	0.11%
700	2.59%	18.98%	6.64%	11.03%	36.17%	24.58%	0.01%	23.12%	5.09%	2.73%	4.29%	38.04%	26.61%	0.12%
800								15.54%	8.36%	3.86%	5.70%	38.75%	27.67%	0.12%
900								11.95%	11.47%	5.15%	7.25%	37.13%	26.93%	0.13%
1000								9.93%	14.62%	6.70%	9.11%	34.33%	25.19%	0.13%
1100								7.94%	18.86%	9.05%	11.99%	29.89%	22.14%	0.13%
T(K)	10 atm							100 atm						
	C ₆ H ₁₃ + C ₂ H ₄	C ₅ H ₁₁ + C ₃ H ₆	CH ₃ + C ₇ H ₁₄	C ₄ H ₉ + C ₄ H ₈	C ₂ H ₅ + C ₆ H ₁₂	C ₃ H ₇ + C ₅ H ₁₀	C ₈ H ₁₆ + H	C ₆ H ₁₃ + C ₂ H ₄	C ₅ H ₁₁ + C ₃ H ₆	CH ₃ + C ₇ H ₁₄	C ₄ H ₉ + C ₄ H ₈	C ₂ H ₅ + C ₆ H ₁₂	C ₃ H ₇ + C ₅ H ₁₀	C ₈ H ₁₆ + H
500	92.60%	0.10%	0.18%	0.34%	4.02%	2.63%	0.13%	99.08%	0.01%	0.02%	0.04%	0.43%	0.28%	0.14%
600	84.62%	0.31%	0.47%	0.79%	8.02%	5.50%	0.29%	97.88%	0.03%	0.06%	0.09%	0.94%	0.65%	0.35%
700	72.05%	0.85%	1.02%	1.55%	14.08%	9.98%	0.47%	95.54%	0.08%	0.14%	0.22%	1.96%	1.39%	0.66%
800	57.97%	1.94%	1.77%	2.52%	20.41%	14.81%	0.60%	91.66%	0.21%	0.32%	0.45%	3.66%	2.67%	1.04%
900	46.74%	3.45%	2.58%	3.48%	24.78%	18.29%	0.67%	86.27%	0.45%	0.61%	0.81%	5.97%	4.45%	1.44%
1000	40.09%	4.90%	3.32%	4.30%	26.69%	19.96%	0.75%	80.25%	0.83%	0.99%	1.25%	8.46%	6.39%	1.82%
1100	37.16%	5.92%	3.89%	4.87%	26.95%	20.36%	0.85%	74.99%	1.29%	1.39%	1.68%	10.47%	8.01%	2.16%
1200	36.51%	6.49%	4.28%	5.23%	26.41%	20.11%	0.97%	71.41%	1.70%	1.73%	2.03%	11.64%	8.99%	2.49%
1300	37.11%	6.75%	4.52%	5.42%	25.53%	19.55%	1.12%	69.58%	1.98%	1.96%	2.24%	12.04%	9.37%	2.83%
1400	38.38%	6.81%	4.66%	5.49%	24.50%	18.87%	1.29%	69.02%	2.11%	2.09%	2.34%	11.92%	9.33%	3.19%
1500	39.49%	6.91%	4.77%	5.57%	23.61%	18.24%	1.42%	69.25%	2.14%	2.14%	2.35%	11.52%	9.06%	3.55%
1600								69.88%	2.11%	2.13%	2.31%	10.98%	8.67%	3.91%
1700								70.70%	2.05%	2.09%	2.24%	10.41%	8.25%	4.27%
1800								71.58%	1.97%	2.03%	2.15%	9.83%	7.82%	4.62%

Table S7. Parameters of the fitted modified Arrhenius expressions, $A \cdot T^\alpha \cdot \exp(-E_a/RT)$, for most important reactions involved in pyrolysis of *n*-decane at pressures of 0.03-0.04, 1, 10, and 100 atm.

The data are presented in the following order:

/ *p*, atm A, cm³ mol⁻¹ s⁻¹ α E_a, cal mol⁻¹/ ! fit btw. *T*₁ and *T*₂ with MAE = mean/max absolute error

The title line for each reaction shows A, α, and E_a at the high-pressure limit.

The fits are provided to a single Arrhenius expression and to a sum of two Arrhenius expressions

C₁₀H₂₂ → C₂H₅ + C₈H₁₇				1.12E+82	-18.19	122300.0
PLOG/3.000E-02	1.33E+120	-30.03	135500.0/	! fit btw. 700 and 2500 K with MAE of 28.1%, 51.1%		
PLOG/1.000E+00	2.39E+110	-26.75	134800.0/	! fit btw. 700 and 2500 K with MAE of 24.7%, 56.7%		
PLOG/1.000E+01	1.12E+98	-22.96	130000.0/	! fit btw. 700 and 2500 K with MAE of 27.1%, 62.9%		
PLOG/1.000E+02	1.12E+82	-18.19	122300.0/	! fit btw. 700 and 2500 K with MAE of 31.2%, 65.2%		
PLOG/3.000E-02	5.32E+271	-68.80	360200.0/			
PLOG/3.000E-02	6.52E+137	-35.11	146300.0/	! fit btw. 700 and 2500 K with MAE of 13.9%, 40.6%		
PLOG/1.000E+00	2.98E+121	-29.80	144000.0/			
PLOG/1.000E+00	2.44E+247	-69.89	180200.0/	! fit btw. 700 and 2500 K with MAE of 16.1%, 34.1%		
PLOG/1.000E+01	2.13E+121	-29.35	149800.0/			
PLOG/1.000E+01	5.68E+206	-56.77	169400.0/	! fit btw. 700 and 2500 K with MAE of 10.5%, 23.4%		
PLOG/1.000E+02	4.91E+118	-28.21	154600.0/			
PLOG/1.000E+02	9.48E+110	-27.58	128600.0/	! fit btw. 700 and 2500 K with MAE of 7.0%, 13.0%		
C₁₀H₂₂ → C₃H₇ + C₇H₁₅				5.47E+82	-18.42	123600.0
PLOG/3.000E-02	7.93E+120	-30.31	136700.0/	! fit btw. 700 and 2500 K with MAE of 28.4%, 52.1%		
PLOG/1.000E+00	1.87E+111	-27.05	136100.0/	! fit btw. 700 and 2500 K with MAE of 24.8%, 56.8%		
PLOG/1.000E+01	7.74E+98	-23.24	131400.0/	! fit btw. 700 and 2500 K with MAE of 27.2%, 63.4%		
PLOG/1.000E+02	5.47E+82	-18.42	123600.0/	! fit btw. 700 and 2500 K with MAE of 31.5%, 66.0%		
PLOG/3.000E-02	8.26E+263	-66.82	350600.0/			
PLOG/3.000E-02	1.30E+139	-35.53	147800.0/	! fit btw. 700 and 2500 K with MAE of 13.8%, 40.2%		
PLOG/1.000E+00	1.50E+122	-30.05	145200.0/			
PLOG/1.000E+00	3.13E+246	-69.69	180400.0/	! fit btw. 700 and 2500 K with MAE of 16.3%, 34.5%		
PLOG/1.000E+01	1.20E+122	-29.61	151100.0/			
PLOG/1.000E+01	1.05E+210	-57.79	171700.0/	! fit btw. 700 and 2500 K with MAE of 10.6%, 23.7%		
PLOG/1.000E+02	2.76E+119	-28.45	155900.0/			

PLOG/1.000E+02	8.80E+111	-27.90	129900.0/	! fit btw. 700 and 2500 K with MAE of 7.1%, 13.1%
C₁₀H₂₂ → C₄H₉ + C₆H₁₃				4.07E+83 -18.64 124800.0
PLOG/3.000E-02	6.39E+121	-30.56	137700.0/	! fit btw. 700 and 2500 K with MAE of 28.7%, 53.0%
PLOG/1.000E+00	1.98E+112	-27.32	137300.0/	! fit btw. 700 and 2500 K with MAE of 24.9%, 56.8%
PLOG/1.000E+01	7.54E+99	-23.50	132600.0/	! fit btw. 700 and 2500 K with MAE of 27.2%, 63.9%
PLOG/1.000E+02	4.07E+83	-18.64	124800.0/	! fit btw. 700 and 2500 K with MAE of 31.7%, 66.7%
PLOG/3.000E-02	2.23E+257	-65.11	342300.0/	
PLOG/3.000E-02	3.23E+140	-35.92	149100.0/	! fit btw. 700 and 2500 K with MAE of 13.7%, 39.7%
PLOG/1.000E+00	9.92E+122	-30.27	146200.0/	
PLOG/1.000E+00	4.21E+245	-69.43	180400.0/	! fit btw. 700 and 2500 K with MAE of 16.5%, 34.9%
PLOG/1.000E+01	8.66E+122	-29.83	152200.0/	
PLOG/1.000E+01	2.78E+213	-58.80	173900.0/	! fit btw. 700 and 2500 K with MAE of 10.8%, 24.1%
PLOG/1.000E+02	3.78E+120	-28.75	157400.0/	
PLOG/1.000E+02	4.16E+111	-27.77	130500.0/	! fit btw. 700 and 2500 K with MAE of 7.2%, 13.1%
C₁₀H₂₂ → C₅H₁₁ + C₅H₁₁				3.08E+83 -18.57 124400.0
PLOG/3.000E-02	4.61E+121	-30.47	137400.0/	! fit btw. 700 and 2500 K with MAE of 28.6%, 52.7%
PLOG/1.000E+00	1.30E+112	-27.23	136900.0/	! fit btw. 700 and 2500 K with MAE of 24.9%, 56.8%
PLOG/1.000E+01	5.15E+99	-23.41	132200.0/	! fit btw. 700 and 2500 K with MAE of 27.2%, 63.7%
PLOG/1.000E+02	3.08E+83	-18.57	124400.0/	! fit btw. 700 and 2500 K with MAE of 31.6%, 66.4%
PLOG/3.000E-02	3.21E+259	-65.63	344800.0/	
PLOG/3.000E-02	1.61E+140	-35.80	148700.0/	! fit btw. 700 and 2500 K with MAE of 13.7%, 39.9%
PLOG/1.000E+00	7.45E+122	-30.19	145800.0/	
PLOG/1.000E+00	1.44E+246	-69.54	180400.0/	! fit btw. 700 and 2500 K with MAE of 16.5%, 34.8%
PLOG/1.000E+01	6.24E+122	-29.75	151800.0/	
PLOG/1.000E+01	3.22E+212	-58.48	173200.0/	! fit btw. 700 and 2500 K with MAE of 10.7%, 23.9%
PLOG/1.000E+02	2.69E+120	-28.67	156900.0/	
PLOG/1.000E+02	2.98E+111	-27.69	130100.0/	! fit btw. 700 and 2500 K with MAE of 7.1%, 13.1%
C₃H₇ (<i>n</i>-propyl) → C₂H₄ + CH₃				3.48E+29 -4.75 38170.0
PLOG/3.950E-02	2.40E+30	-5.95	32650.0/	! fit btw. 500 and 2500 K with MAE of 18.1%, 43.6%
PLOG/1.000E+00	4.04E+33	-6.44	36730.0/	! fit btw. 500 and 2500 K with MAE of 13.6%, 24.6%

PLOG/1.000E+01	2.21E+33	-6.08	38490.0/	! fit btw. 500 and 2500 K with MAE of 8.0%, 16.6%
PLOG/1.000E+02	3.48E+29	-4.75	38170.0/	! fit btw. 500 and 2500 K with MAE of 6.4%, 17.8%
PLOG/3.950E-02	1.97E+58	-14.32	45690.0/	
PLOG/3.950E-02	3.73E+20	-3.12	28930.0/	! fit btw. 500 and 2500 K with MAE of 0.8%, 1.6%
PLOG/1.000E+00	3.00E+43	-9.37	41490.0/	
PLOG/1.000E+00	1.16E+45	-9.07	65950.0/	! fit btw. 500 and 2500 K with MAE of 1.9%, 7.5%
PLOG/1.000E+01	3.47E+36	-7.02	40090.0/	
PLOG/1.000E+01	6.69E+112	-26.38	162600.0/	! fit btw. 500 and 2500 K with MAE of 3.4%, 11.1%
PLOG/1.000E+02	3.17E+63	-14.52	61280.0/	
PLOG/1.000E+02	5.53E+23	-3.14	34690.0/	! fit btw. 500 and 2500 K with MAE of 0.5%, 1.1%

C₃H₇ (*n*-propyl) → C₃H₆ + H

9.95E+30 -5.30 43000.0

PLOG/3.950E-02	1.76E+26	-5.14	34020.0/	! fit btw. 500 and 2500 K with MAE of 20.5%, 52.0%
PLOG/1.000E+00	6.65E+32	-6.49	39650.0/	! fit btw. 500 and 2500 K with MAE of 16.0%, 29.3%
PLOG/1.000E+01	1.72E+34	-6.54	42600.0/	! fit btw. 500 and 2500 K with MAE of 9.6%, 20.3%
PLOG/1.000E+02	9.95E+30	-5.30	43000.0/	! fit btw. 500 and 2500 K with MAE of 6.7%, 17.6%

PLOG/3.950E-02	3.44E+53	-13.32	46630.0/	
PLOG/3.950E-02	8.17E+15	-2.14	30670.0/	! fit btw. 500 and 2500 K with MAE of 1.1%, 2.2%
PLOG/1.000E+00	7.94E+45	-10.38	45880.0/	
PLOG/1.000E+00	7.95E+33	-6.39	55110.0/	! fit btw. 500 and 2500 K with MAE of 1.6%, 5.8%
PLOG/1.000E+01	7.19E+38	-7.90	44910.0/	
PLOG/1.000E+01	2.96E+104	-24.48	151300.0/	! fit btw. 500 and 2500 K with MAE of 3.0%, 10.1%
PLOG/1.000E+02	9.25E+63	-14.81	64840.0/	
PLOG/1.000E+02	2.51E+24	-3.46	39100.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 1.5%

C₄H₉ (1-butyl) → C₂H₄ + C₂H₅

1.54E+31 -5.17 37980.0

PLOG/3.950E-02	1.57E+30	-5.87	31080.0/	! fit btw. 500 and 2500 K with MAE of 22.1%, 62.8%
PLOG/1.000E+00	2.79E+34	-6.65	35940.0/	! fit btw. 500 and 2500 K with MAE of 17.5%, 31.6%
PLOG/1.000E+01	4.53E+34	-6.42	38050.0/	! fit btw. 500 and 2500 K with MAE of 10.6%, 21.0%
PLOG/1.000E+02	1.54E+31	-5.17	37980.0/	! fit btw. 500 and 2500 K with MAE of 7.1%, 18.5%

PLOG/3.950E-02	2.30E+62	-15.53	45690.0/	
PLOG/3.950E-02	1.19E+22	-3.48	29290.0/	! fit btw. 500 and 2500 K with MAE of 1.6%, 2.9%
PLOG/1.000E+00	1.47E+49	-11.02	42940.0/	
PLOG/1.000E+00	3.49E+37	-7.10	52910.0/	! fit btw. 500 and 2500 K with MAE of 2.1%, 9.4%

PLOG/1.000E+01	5.45E+39	-7.91	40580.0/	
PLOG/1.000E+01	5.25E+87	-19.84	125300.0/	! fit btw. 500 and 2500 K with MAE of 3.7%, 13.2%
PLOG/1.000E+02	3.12E+70	-16.51	63750.0/	
PLOG/1.000E+02	6.18E+24	-3.39	34230.0/	! fit btw. 500 and 2500 K with MAE of 0.6%, 1.5%

C₄H₉ (1-butyl) → C₄H₈ (1-butene) + H

1.86E+33 -5.98 44880.0

PLOG/3.950E-02	6.33E+24	-4.84	32880.0/	! fit btw. 500 and 2500 K with MAE of 26.5%, 80.8%
PLOG/1.000E+00	5.77E+33	-6.84	40270.0/	! fit btw. 500 and 2500 K with MAE of 21.7%, 47.6%
PLOG/1.000E+01	1.49E+36	-7.15	44050.0/	! fit btw. 500 and 2500 K with MAE of 14.0%, 26.5%
PLOG/1.000E+02	1.86E+33	-5.98	44880.0/	! fit btw. 500 and 2500 K with MAE of 8.1%, 18.9%

PLOG/3.950E-02	1.14E+59	-15.12	48510.0/	
PLOG/3.950E-02	1.21E+16	-2.26	31610.0/	! fit btw. 500 and 2500 K with MAE of 2.5%, 5.3%
PLOG/1.000E+00	2.17E+54	-12.97	49910.0/	
PLOG/1.000E+00	5.93E+28	-5.17	46650.0/	! fit btw. 500 and 2500 K with MAE of 2.0%, 7.3%
PLOG/1.000E+01	1.19E+44	-9.48	47940.0/	
PLOG/1.000E+01	7.11E+66	-14.71	101300.0/	! fit btw. 500 and 2500 K with MAE of 3.3%, 12.8%
PLOG/1.000E+02	2.65E+73	-17.59	70430.0/	
PLOG/1.000E+02	6.29E+25	-3.88	40560.0/	! fit btw. 500 and 2500 K with MAE of 0.8%, 2.4%

C₅H₁₁ (1-pentyl) → C₂H₄ + C₃H₇

7.58E+29 -4.81 37810.0

PLOG/3.000E-02	1.21E+24	-4.21	28160.0/	! fit btw. 500 and 2500 K with MAE of 21.4%, 67.1%
PLOG/3.947E-02	9.99E+24	-4.43	28810.0/	! fit btw. 500 and 2500 K with MAE of 21.4%, 65.9%
PLOG/1.000E+00	1.67E+33	-6.31	35790.0/	! fit btw. 500 and 2500 K with MAE of 17.4%, 32.0%
PLOG/1.000E+01	9.37E+33	-6.23	38260.0/	! fit btw. 500 and 2500 K with MAE of 9.8%, 19.7%
PLOG/1.000E+02	7.58E+29	-4.81	37810.0/	! fit btw. 500 and 2500 K with MAE of 7.1%, 19.4%

PLOG/3.000E-02	7.95E+56	-14.09	42830.0/	
PLOG/3.000E-02	3.38E+18	-2.53	28380.0/	! fit btw. 500 and 2500 K with MAE of 2.1%, 3.9%
PLOG/3.947E-02	2.02E+57	-14.16	43270.0/	
PLOG/3.947E-02	1.46E+19	-2.67	28850.0/	! fit btw. 500 and 2500 K with MAE of 1.9%, 3.6%
PLOG/1.000E+00	1.94E+48	-10.79	42930.0/	
PLOG/1.000E+00	7.83E+34	-6.39	50730.0/	! fit btw. 500 and 2500 K with MAE of 2.1%, 9.2%
PLOG/1.000E+01	1.60E+38	-7.47	40380.0/	
PLOG/1.000E+01	3.13E+102	-23.67	146700.0/	! fit btw. 500 and 2500 K with MAE of 4.1%, 13.4%
PLOG/1.000E+02	9.70E+66	-15.47	63000.0/	
PLOG/1.000E+02	5.75E+23	-3.11	34140.0/	! fit btw. 500 and 2500 K with MAE of 0.6%, 1.5%

C₅H₁₁ (1-pentyl) → C₃H₆ + C₂H₅				3.24E+41	-8.24	50560.0
PLOG/3.000E-02	3.80E+33	-6.90	32530.0/	! fit btw. 500 and 2500 K with MAE of 26.0%, 80.0%		
PLOG/3.947E-02	6.35E+34	-7.22	33500.0/	! fit btw. 500 and 2500 K with MAE of 25.9%, 78.2%		
PLOG/1.000E+00	6.41E+45	-9.97	44340.0/	! fit btw. 500 and 2500 K with MAE of 23.0%, 37.8%		
PLOG/1.000E+01	7.13E+47	-10.28	49770.0/	! fit btw. 500 and 2500 K with MAE of 16.4%, 35.4%		
PLOG/1.000E+02	3.24E+41	-8.24	50560.0/	! fit btw. 500 and 2500 K with MAE of 20.0%, 72.8%		
PLOG/3.000E-02	6.76E+67	-17.17	48140.0/			
PLOG/3.000E-02	1.16E+25	-4.38	31280.0/	! fit btw. 500 and 2500 K with MAE of 3.1%, 7.9%		
PLOG/3.947E-02	1.88E+69	-17.56	49220.0/			
PLOG/3.947E-02	1.43E+26	-4.66	32040.0/	! fit btw. 500 and 2500 K with MAE of 2.7%, 6.0%		
PLOG/1.000E+00	5.54E+62	-14.98	52510.0/			
PLOG/1.000E+00	9.38E+57	-12.74	74050.0/	! fit btw. 500 and 2500 K with MAE of 4.2%, 18.7%		
PLOG/1.000E+01	4.00E+197	-48.92	262600.0/			
PLOG/1.000E+01	3.42E+52	-11.65	52130.0/	! fit btw. 500 and 2500 K with MAE of 9.7%, 36.1%		
PLOG/1.000E+02	4.64E+51	-11.05	58310.0/			
PLOG/1.000E+02	7.14E+191	-56.71	94700.0/	! fit btw. 500 and 2500 K with MAE of 7.9%, 17.4%		
C₅H₁₁ (1-pentyl) → C₅H₁₀ (1-pentene) + H				4.87E+31	-5.55	44230.0
PLOG/3.000E-02	1.79E+20	-3.59	30630.0/	! fit btw. 500 and 2500 K with MAE of 25.9%, 85.3%		
PLOG/3.947E-02	3.55E+21	-3.91	31430.0/	! fit btw. 500 and 2500 K with MAE of 25.7%, 83.5%		
PLOG/1.000E+00	3.71E+33	-6.78	40500.0/	! fit btw. 500 and 2500 K with MAE of 21.2%, 45.3%		
PLOG/1.000E+01	6.93E+35	-7.05	44240.0/	! fit btw. 500 and 2500 K with MAE of 12.3%, 24.2%		
PLOG/1.000E+02	4.87E+31	-5.55	44230.0/	! fit btw. 500 and 2500 K with MAE of 8.1%, 21.9%		
PLOG/3.000E-02	2.78E+56	-14.46	46980.0/			
PLOG/3.000E-02	2.45E+13	-1.53	30440.0/	! fit btw. 500 and 2500 K with MAE of 3.2%, 6.0%		
PLOG/3.947E-02	1.66E+57	-14.62	47560.0/			
PLOG/3.947E-02	3.41E+14	-1.81	31160.0/	! fit btw. 500 and 2500 K with MAE of 3.0%, 5.7%		
PLOG/1.000E+00	2.59E+53	-12.69	49820.0/			
PLOG/1.000E+00	3.86E+30	-5.63	49260.0/	! fit btw. 500 and 2500 K with MAE of 2.1%, 8.0%		
PLOG/1.000E+01	7.97E+41	-8.84	47250.0/			
PLOG/1.000E+01	1.14E+85	-19.44	126800.0/	! fit btw. 500 and 2500 K with MAE of 4.1%, 14.6%		
PLOG/1.000E+02	1.69E+70	-16.63	69980.0/			
PLOG/1.000E+02	3.73E+24	-3.57	40010.0/	! fit btw. 500 and 2500 K with MAE of 0.7%, 1.7%		

C₅H₁₁ (2-pentyl) → C₂H₄ + C₃H₇				5.00E+45	-9.51	56570.0
PLOG/3.000E-02	4.59E+38	-8.58	38250.0/	! fit btw. 500 and 2500 K with MAE of 28.1%, 89.1%		
PLOG/3.947E-02	4.24E+39	-8.81	39100.0/	! fit btw. 500 and 2500 K with MAE of 28.4%, 88.5%		
PLOG/1.000E+00	2.60E+50	-11.43	50100.0/	! fit btw. 500 and 2500 K with MAE of 26.0%, 43.6%		
PLOG/1.000E+01	2.90E+52	-11.70	55770.0/	! fit btw. 500 and 2500 K with MAE of 18.2%, 36.7%		
PLOG/1.000E+02	5.00E+45	-9.51	56570.0/	! fit btw. 500 and 2500 K with MAE of 20.1%, 73.6%		
PLOG/3.000E-02	1.39E+79	-20.73	56630.0/			
PLOG/3.000E-02	3.96E+30	-6.19	36910.0/	! fit btw. 500 and 2500 K with MAE of 2.3%, 4.4%		
PLOG/3.947E-02	3.42E+79	-20.78	57310.0/			
PLOG/3.947E-02	5.11E+30	-6.19	37210.0/	! fit btw. 500 and 2500 K with MAE of 2.4%, 4.4%		
PLOG/1.000E+00	5.44E+69	-17.16	59410.0/			
PLOG/1.000E+00	6.35E+58	-13.19	75680.0/	! fit btw. 500 and 2500 K with MAE of 4.7%, 20.7%		
PLOG/1.000E+01	2.01E+58	-13.42	58700.0/			
PLOG/1.000E+01	1.09E+150	-36.63	204000.0/	! fit btw. 500 and 2500 K with MAE of 10.0%, 38.1%		
PLOG/1.000E+02	1.93E+195	-57.79	100200.0/			
PLOG/1.000E+02	3.87E+55	-12.25	64110.0/	! fit btw. 500 and 2500 K with MAE of 8.7%, 19.4%		
C₅H₁₁ (2-pentyl) → C₃H₆ + C₂H₅				1.24E+30	-4.86	38050.0
PLOG/3.000E-02	2.48E+31	-6.23	31990.0/	! fit btw. 500 and 2500 K with MAE of 25.0%, 73.7%		
PLOG/3.947E-02	6.51E+31	-6.31	32430.0/	! fit btw. 500 and 2500 K with MAE of 24.8%, 71.2%		
PLOG/1.000E+00	4.14E+35	-6.96	37300.0/	! fit btw. 500 and 2500 K with MAE of 17.9%, 29.9%		
PLOG/1.000E+01	6.43E+34	-6.44	38890.0/	! fit btw. 500 and 2500 K with MAE of 10.1%, 19.5%		
PLOG/1.000E+02	1.24E+30	-4.86	38050.0/	! fit btw. 500 and 2500 K with MAE of 7.5%, 20.7%		
PLOG/3.000E-02	2.49E+67	-17.04	48390.0/			
PLOG/3.000E-02	6.49E+22	-3.70	30020.0/	! fit btw. 500 and 2500 K with MAE of 1.9%, 3.2%		
PLOG/3.947E-02	2.19E+67	-16.97	48700.0/			
PLOG/3.947E-02	3.76E+22	-3.61	29910.0/	! fit btw. 500 and 2500 K with MAE of 1.9%, 3.4%		
PLOG/1.000E+00	8.30E+48	-10.90	43710.0/			
PLOG/1.000E+00	1.05E+46	-9.29	64690.0/	! fit btw. 500 and 2500 K with MAE of 3.0%, 12.5%		
PLOG/1.000E+01	4.43E+38	-7.57	40810.0/			
PLOG/1.000E+01	1.22E+120	-28.24	170100.0/	! fit btw. 500 and 2500 K with MAE of 4.8%, 16.0%		
PLOG/1.000E+02	3.50E+67	-15.60	63650.0/			
PLOG/1.000E+02	5.69E+23	-3.09	34250.0/	! fit btw. 500 and 2500 K with MAE of 0.6%, 1.4%		

C₆H₁₃ (1-hexyl) → C₂H₄ + C₄H₉				1.59E+28	-4.34	36860.0
PLOG/3.000E-02	7.72E-07	5.74	22600.0/	! fit btw. 500 and 800 K with MAE of 2.7%, 4.5%		
PLOG/3.947E-02	3.27E+00	3.66	24730.0/	! fit btw. 500 and 800 K with MAE of 1.3%, 2.2%		
PLOG/1.000E+00	7.76E+31	-5.97	35400.0/	! fit btw. 500 and 1200 K with MAE of 0.4%, 1.0%		
PLOG/1.000E+01	2.76E+34	-6.42	38240.0/	! fit btw. 500 and 1600 K with MAE of 3.5%, 7.9%		
PLOG/1.000E+02	1.59E+28	-4.34	36860.0/	! fit btw. 500 and 2000 K with MAE of 7.3%, 15.8%		
PLOG/3.000E-02	7.72E-07	5.74	22600.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 2.7%, 4.5%		
PLOG/3.947E-02	3.27E+00	3.66	24730.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 1.3%, 2.2%		
PLOG/1.000E+00	1.16E+39	-8.22	38530.0/			
PLOG/1.000E+00	2.19E+22	-3.18	31520.0/	! fit btw. 500 and 1200 K with MAE of 0.3%, 0.6%		
PLOG/1.000E+01	2.50E+72	-17.65	60000.0/			
PLOG/1.000E+01	6.80E+28	-4.81	35280.0/	! fit btw. 500 and 1600 K with MAE of 0.2%, 0.4%		
PLOG/1.000E+02	2.16E+60	-13.58	58990.0/			
PLOG/1.000E+02	2.66E+23	-3.03	33900.0/	! fit btw. 500 and 2000 K with MAE of 0.4%, 0.9%		
C₆H₁₃ (1-hexyl) → C₃H₆ + C₃H₇				1.44E+38	-7.24	46910.0
PLOG/3.000E-02	5.23E-02	4.46	23000.0/	! fit btw. 500 and 800 K with MAE of 2.9%, 4.9%		
PLOG/3.947E-02	1.02E+08	1.57	26410.0/	! fit btw. 500 and 800 K with MAE of 1.7%, 2.9%		
PLOG/1.000E+00	1.13E+43	-8.97	42720.0/	! fit btw. 500 and 1200 K with MAE of 3.6%, 8.4%		
PLOG/1.000E+01	1.12E+47	-9.97	47900.0/	! fit btw. 500 and 1600 K with MAE of 13.7%, 28.7%		
PLOG/1.000E+02	1.44E+38	-7.24	46910.0/	! fit btw. 500 and 2000 K with MAE of 23.0%, 57.5%		
PLOG/3.000E-02	5.23E-02	4.46	23000.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 2.9%, 4.9%		
PLOG/3.947E-02	1.02E+08	1.57	26410.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 1.7%, 2.9%		
PLOG/1.000E+00	6.11E-15	-8.27	-82600.0/			
PLOG/1.000E+00	7.82E+47	-10.40	45210.0/	! fit btw. 500 and 1200 K with MAE of 1.2%, 2.1%		
PLOG/1.000E+01	9.15E+64	-15.11	59250.0/			
PLOG/1.000E+01	8.32E+42	-9.44	41580.0/	! fit btw. 500 and 1600 K with MAE of 2.4%, 4.5%		
PLOG/1.000E+02	1.70E+76	-18.04	73250.0/			
PLOG/1.000E+02	6.54E+24	-3.59	38460.0/	! fit btw. 500 and 2000 K with MAE of 1.5%, 3.8%		



2.53E+38 -7.35 50080.0

PLOG/3.000E-02	3.62E-17	9.38	21720.0/	! fit btw. 500 and 800 K with MAE of 4.8%, 8.2%
PLOG/3.947E-02	8.60E-05	5.50	26180.0/	! fit btw. 500 and 800 K with MAE of 2.8%, 4.7%
PLOG/1.000E+00	4.70E+39	-8.03	44160.0/	! fit btw. 500 and 1200 K with MAE of 5.5%, 11.7%
PLOG/1.000E+01	2.86E+47	-10.18	50840.0/	! fit btw. 500 and 1600 K with MAE of 15.6%, 32.7%
PLOG/1.000E+02	2.53E+38	-7.35	50080.0/	! fit btw. 500 and 2000 K with MAE of 25.8%, 67.4%

PLOG/3.000E-02	3.62E-17	9.38	21720.0/	
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 4.8%, 8.2%
PLOG/3.947E-02	8.60E-05	5.50	26180.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 2.8%, 4.7%
PLOG/1.000E+00	4.26E+04	-17.94	-96180.0/	
PLOG/1.000E+00	8.61E+46	-10.18	47890.0/	! fit btw. 500 and 1200 K with MAE of 1.4%, 3.9%
PLOG/1.000E+01	1.24E+11	-2.80	13530.0/	
PLOG/1.000E+01	4.71E+52	-11.67	54140.0/	! fit btw. 500 and 1600 K with MAE of 7.5%, 15.7%
PLOG/1.000E+02	2.47E+78	-18.70	77570.0/	
PLOG/1.000E+02	6.38E+22	-3.06	40360.0/	! fit btw. 500 and 2000 K with MAE of 1.7%, 4.4%



3.23E+38 -7.40 50990.0

PLOG/3.000E-02	2.52E-15	8.74	23020.0/	! fit btw. 500 and 800 K with MAE of 4.9%, 8.3%
PLOG/3.947E-02	6.84E-03	4.85	27540.0/	! fit btw. 500 and 800 K with MAE of 2.9%, 4.8%
PLOG/1.000E+00	1.04E+40	-8.18	45030.0/	! fit btw. 500 and 1200 K with MAE of 5.5%, 11.6%
PLOG/1.000E+01	4.82E+47	-10.28	51720.0/	! fit btw. 500 and 1600 K with MAE of 15.5%, 32.6%
PLOG/1.000E+02	3.23E+38	-7.40	50990.0/	! fit btw. 500 and 2000 K with MAE of 25.9%, 68.0%

PLOG/3.000E-02	2.52E-15	8.74	23020.0/	
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 4.9%, 8.3%
PLOG/3.947E-02	6.84E-03	4.85	27540.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 2.9%, 4.8%
PLOG/1.000E+00	6.63E+03	-1.60	3955.0/	
PLOG/1.000E+00	7.14E+45	-9.90	48060.0/	! fit btw. 500 and 1200 K with MAE of 1.6%, 3.6%
PLOG/1.000E+01	1.92E+10	-2.80	12600.0/	
PLOG/1.000E+01	6.05E+52	-11.74	54950.0/	! fit btw. 500 and 1600 K with MAE of 7.5%, 15.6%
PLOG/1.000E+02	4.49E+78	-18.79	78570.0/	
PLOG/1.000E+02	6.15E+22	-3.08	41200.0/	! fit btw. 500 and 2000 K with MAE of 1.7%, 4.4%

C₆H₁₃ (1-hexyl) → C₆H₁₂ (1-hexene) + H				8.85E+29	-5.03	43290.0
PLOG/3.000E-02	2.78E+04	2.11	31380.0/	! fit btw. 500 and 800 K with MAE of 3.3%, 5.6%		
PLOG/3.947E-02	1.68E+13	-0.61	34550.0/	! fit btw. 500 and 800 K with MAE of 2.0%, 3.3%		
PLOG/1.000E+00	1.04E+34	-6.89	41480.0/	! fit btw. 500 and 1200 K with MAE of 0.9%, 1.6%		
PLOG/1.000E+01	1.61E+37	-7.48	44740.0/	! fit btw. 500 and 1600 K with MAE of 3.7%, 8.6%		
PLOG/1.000E+02	8.85E+29	-5.03	43290.0/	! fit btw. 500 and 2000 K with MAE of 8.3%, 18.6%		
PLOG/3.000E-02	2.78E+04	2.11	31380.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 3.3%, 5.6%		
PLOG/3.947E-02	1.68E+13	-0.61	34550.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 2.0%, 3.3%		
PLOG/1.000E+00	7.48E+32	-7.98	34520.0/			
PLOG/1.000E+00	2.53E+35	-7.30	42230.0/	! fit btw. 500 and 1200 K with MAE of 0.6%, 1.3%		
PLOG/1.000E+01	3.86E+40	-8.45	46780.0/			
PLOG/1.000E+01	1.91E+136	-40.26	70030.0/	! fit btw. 500 and 1600 K with MAE of 1.3%, 3.2%		
PLOG/1.000E+02	4.27E+63	-14.71	66220.0/			
PLOG/1.000E+02	1.62E+24	-3.45	39780.0/	! fit btw. 500 and 2000 K with MAE of 0.5%, 1.0%		
C₆H₁₃ (2-hexyl) → C₂H₄ + C₄H₉				1.61E+37	-7.00	50200.0
PLOG/3.000E-02	3.02E+57	-14.14	46850.0/	! fit btw. 500 and 1200 K with MAE of 8.0%, 28.2%		
PLOG/3.947E-02	2.49E+59	-14.66	48050.0/	! fit btw. 500 and 1200 K with MAE of 5.2%, 16.9%		
PLOG/1.000E+00	2.32E+54	-12.54	50730.0/	! fit btw. 500 and 1500 K with MAE of 11.1%, 40.5%		
PLOG/1.000E+01	5.59E+49	-10.84	52780.0/	! fit btw. 500 and 1700 K with MAE of 20.4%, 43.7%		
PLOG/1.000E+02	1.61E+37	-7.00	50200.0/	! fit btw. 500 and 2100 K with MAE of 32.1%, 82.0%		
PLOG/3.000E-02	4.74E+102	-28.26	63080.0/			
PLOG/3.000E-02	2.59E+109	-29.04	80300.0/	! fit btw. 500 and 1200 K with MAE of 7.5%, 17.8%		
PLOG/3.947E-02	4.27E+90	-24.48	58910.0/			
PLOG/3.947E-02	2.58E+88	-22.92	67990.0/	! fit btw. 500 and 1200 K with MAE of 5.0%, 12.9%		
PLOG/1.000E+00	6.08E+53	-11.31	76380.0/			
PLOG/1.000E+00	1.11E+58	-13.66	52230.0/	! fit btw. 500 and 1500 K with MAE of 9.3%, 29.9%		
PLOG/1.000E+01	2.29E+54	-12.16	55590.0/			
PLOG/1.000E+01	1.07E+35	-13.98	392.8/	! fit btw. 500 and 1700 K with MAE of 15.7%, 46.1%		
PLOG/1.000E+02	1.72E+41	-8.13	53030.0/			
PLOG/1.000E+02	2.34E+16	-3.20	26210.0/	! fit btw. 500 and 2100 K with MAE of 25.7%, 74.8%		

C₆H₁₃ (2-hexyl) → C₃H₆ + C₃H₇				1.77E+29	-4.60	38210.0
PLOG/3.000E-02	1.04E+55	-13.22	43900.0/	! fit btw. 500 and 1200 K with MAE of 7.0%, 24.8%		
PLOG/3.947E-02	2.41E+56	-13.58	44800.0/	! fit btw. 500 and 1200 K with MAE of 4.3%, 14.6%		
PLOG/1.000E+00	1.84E+46	-10.09	43160.0/	! fit btw. 500 and 1500 K with MAE of 6.2%, 14.2%		
PLOG/1.000E+01	5.54E+37	-7.29	40990.0/	! fit btw. 500 and 1700 K with MAE of 8.5%, 18.5%		
PLOG/1.000E+02	1.77E+29	-4.60	38210.0/	! fit btw. 500 and 2100 K with MAE of 10.0%, 23.2%		
PLOG/3.000E-02	6.12E+91	-24.72	57040.0/			
PLOG/3.000E-02	7.68E+105	-27.80	76980.0/	! fit btw. 500 and 1200 K with MAE of 6.9%, 16.7%		
PLOG/3.947E-02	6.91E+76	-20.02	51860.0/			
PLOG/3.947E-02	1.20E+86	-22.02	65760.0/	! fit btw. 500 and 1200 K with MAE of 4.6%, 11.7%		
PLOG/1.000E+00	2.02E+49	-10.97	44900.0/			
PLOG/1.000E+00	1.05E+31	-13.31	-10360.0/	! fit btw. 500 and 1500 K with MAE of 4.6%, 16.1%		
PLOG/1.000E+01	5.28E+70	-16.86	61700.0/			
PLOG/1.000E+01	4.49E+29	-5.03	36290.0/	! fit btw. 500 and 1700 K with MAE of 0.8%, 3.1%		
PLOG/1.000E+02	1.14E+42	-8.17	48140.0/			
PLOG/1.000E+02	1.56E+43	-9.38	40480.0/	! fit btw. 500 and 2100 K with MAE of 1.6%, 6.1%		
C₆H₁₃ (2-hexyl) → C₄H₈ (1-butene) + C₂H₅				8.26E+47	-10.24	62600.0
PLOG/3.000E-02	1.65E+66	-16.65	51670.0/	! fit btw. 500 and 1200 K with MAE of 25.1%, 109.5%		
PLOG/3.947E-02	4.08E+73	-18.80	55530.0/	! fit btw. 500 and 1200 K with MAE of 12.0%, 46.4%		
PLOG/1.000E+00	3.88E+69	-17.08	60780.0/	! fit btw. 500 and 1500 K with MAE of 52.3%, 335.2%		
PLOG/1.000E+01	7.38E+71	-17.44	68280.0/	! fit btw. 500 and 1700 K with MAE of 41.8%, 127.8%		
PLOG/1.000E+02	8.26E+47	-10.24	62600.0/	! fit btw. 500 and 2100 K with MAE of 85.3%, 365.8%		
PLOG/3.000E-02	3.34E+65	-16.26	58130.0/			
PLOG/3.000E-02	8.91E+68	-17.51	52590.0/	! fit btw. 500 and 1200 K with MAE of 25.4%, 107.5%		
PLOG/3.947E-02	1.31E+73	-18.51	61530.0/			
PLOG/3.947E-02	2.96E+76	-19.71	56520.0/	! fit btw. 500 and 1200 K with MAE of 12.0%, 45.8%		
PLOG/1.000E+00	5.64E+68	-15.33	93230.0/			
PLOG/1.000E+00	9.33E+72	-18.15	61790.0/	! fit btw. 500 and 1500 K with MAE of 44.9%, 255.4%		
PLOG/1.000E+01	7.81E+80	-20.03	73790.0/			
PLOG/1.000E+01	3.77E+57	-20.49	16830.0/	! fit btw. 500 and 1700 K with MAE of 31.7%, 112.8%		
PLOG/1.000E+02	7.94E+07	-21.42	-98190.0/			
PLOG/1.000E+02	2.85E+55	-12.37	67710.0/	! fit btw. 500 and 2100 K with MAE of 71.1%, 320.9%		

C₆H₁₃ (2-hexyl) → C₅H₁₀ (1-pentene) + CH₃				7.80E+47	-10.25	63360.0
PLOG/3.000E-02	2.38E+66	-16.77	52300.0/	! fit btw. 500 and 1200 K with MAE of 24.4%, 105.5%		
PLOG/3.947E-02	3.67E+73	-18.86	56070.0/	! fit btw. 500 and 1200 K with MAE of 11.8%, 45.5%		
PLOG/1.000E+00	8.90E+69	-17.23	61590.0/	! fit btw. 500 and 1500 K with MAE of 49.1%, 307.9%		
PLOG/1.000E+01	2.35E+54	-12.26	60830.0/	! fit btw. 500 and 1800 K with MAE of 73.3%, 366.0%		
PLOG/1.000E+02	7.04E+48	-10.59	63570.0/	! fit btw. 500 and 2200 K with MAE of 82.4%, 367.6%		
PLOG/3.000E-02	4.09E+65	-16.35	58900.0/			
PLOG/3.000E-02	1.16E+69	-17.62	53200.0/	! fit btw. 500 and 1200 K with MAE of 24.7%, 103.9%		
PLOG/3.947E-02	1.72E+129	-36.23	76230.0/			
PLOG/3.947E-02	1.69E+151	-41.25	104300.0/	! fit btw. 500 and 1200 K with MAE of 11.6%, 25.7%		
PLOG/1.000E+00	7.22E+68	-15.42	93700.0/			
PLOG/1.000E+00	1.23E+73	-18.23	62500.0/	! fit btw. 500 and 1500 K with MAE of 42.5%, 236.3%		
PLOG/1.000E+01	4.69E+80	-20.00	74370.0/			
PLOG/1.000E+01	6.79E+57	-20.59	17690.0/	! fit btw. 500 and 1700 K with MAE of 30.8%, 107.1%		
PLOG/1.000E+02	1.13E+08	-13.16	-45930.0/			
PLOG/1.000E+02	3.24E+55	-12.40	68530.0/	! fit btw. 500 and 2100 K with MAE of 69.4%, 307.7%		
C₆H₁₃ (3-hexyl) → C₂H₄ + C₄H₉				6.10E+43	-8.99	56400.0
PLOG/3.000E-02	1.22E+58	-14.34	49390.0/	! fit btw. 500 and 1300 K with MAE of 27.3%, 58.6%		
PLOG/3.947E-02	3.48E+57	-14.12	49610.0/	! fit btw. 500 and 1300 K with MAE of 27.7%, 62.0%		
PLOG/1.000E+00	9.07E+61	-14.92	56680.0/	! fit btw. 500 and 1500 K with MAE of 8.8%, 20.3%		
PLOG/1.000E+01	3.90E+52	-11.78	56760.0/	! fit btw. 500 and 1700 K with MAE of 20.5%, 36.5%		
PLOG/1.000E+02	6.10E+43	-8.99	56400.0/	! fit btw. 500 and 2000 K with MAE of 26.4%, 70.7%		
PLOG/3.947E-02	4.79E+79	-20.85	58880.0/			
PLOG/3.947E-02	1.32E+56	-9.31	128900.0/	! fit btw. 500 and 1300 K with MAE of 2.2%, 6.3%		
PLOG/1.000E-01	1.29E+184	-47.95	180000.0/			
PLOG/1.000E-01	8.99E+74	-19.24	58380.0/	! fit btw. 500 and 1300 K with MAE of 3.1%, 10.6%		
PLOG/1.000E+00	3.31E+21	-16.10	-41960.0/			
PLOG/1.000E+00	2.40E+65	-15.91	58640.0/	! fit btw. 500 and 1500 K with MAE of 7.0%, 22.6%		
PLOG/1.000E+01	3.19E+56	-12.95	58560.0/			
PLOG/1.000E+01	2.41E+71	3.05	576700.0/	! fit btw. 500 and 1700 K with MAE of 15.3%, 36.7%		
PLOG/1.000E+02	4.22E+85	-20.87	84980.0/			
PLOG/1.000E+02	1.28E+27	-4.38	46170.0/	! fit btw. 500 and 2000 K with MAE of 1.7%, 4.6%		

C₆H₁₃ (3-hexyl) → C₃H₆ + C₃H₇				2.39E+60	-13.87	69370.0
PLOG/3.000E-02	1.07E+59	-14.40	49060.0/	! fit btw. 500 and 1300 K with MAE of 34.7%, 82.8%		
PLOG/3.947E-02	5.71E+58	-14.27	49520.0/	! fit btw. 500 and 1300 K with MAE of 36.1%, 89.7%		
PLOG/1.000E+00	1.89E+81	-20.53	66680.0/	! fit btw. 500 and 1500 K with MAE of 12.2%, 30.9%		
PLOG/1.000E+01	2.03E+77	-19.02	71370.0/	! fit btw. 500 and 1600 K with MAE of 27.2%, 62.1%		
PLOG/1.000E+02	2.39E+60	-13.87	69370.0/	! fit btw. 500 and 2000 K with MAE of 44.5%, 135.6%		
PLOG/3.000E-02	2.57E+86	-22.73	60530.0/			
PLOG/3.000E-02	3.92E-10	9.72	86930.0/	! fit btw. 500 and 1300 K with MAE of 2.0%, 5.0%		
PLOG/3.947E-02	4.15E+86	-22.74	61200.0/			
PLOG/3.947E-02	7.23E+57	-8.92	141200.0/	! fit btw. 500 and 1300 K with MAE of 2.2%, 6.4%		
PLOG/1.000E+00	5.81E+86	-22.12	69820.0/			
PLOG/1.000E+00	5.36E+65	-24.17	9371.0/	! fit btw. 500 and 1500 K with MAE of 9.4%, 35.3%		
PLOG/1.000E+01	4.22E+85	-21.40	76670.0/			
PLOG/1.000E+01	2.49E+52	-15.88	33580.0/	! fit btw. 500 and 1600 K with MAE of 13.2%, 28.7%		
PLOG/1.000E+02	5.13E+35	-7.08	54050.0/			
PLOG/1.000E+02	1.09E+111	-28.20	104200.0/	! fit btw. 500 and 2000 K with MAE of 3.5%, 10.3%		
C₆H₁₃ (3-hexyl) → C₄H₈ (1-butene) + C₂H₅				2.39E+29	-4.68	37850.0
PLOG/3.000E-02	4.66E+66	-16.78	48400.0/	! fit btw. 500 and 1300 K with MAE of 6.9%, 21.8%		
PLOG/3.947E-02	9.38E+66	-16.82	48810.0/	! fit btw. 500 and 1300 K with MAE of 7.6%, 24.4%		
PLOG/1.000E+00	1.74E+48	-10.70	43760.0/	! fit btw. 500 and 1500 K with MAE of 5.8%, 14.4%		
PLOG/1.000E+01	2.56E+38	-7.52	40920.0/	! fit btw. 500 and 1700 K with MAE of 8.5%, 18.7%		
PLOG/1.000E+02	2.39E+29	-4.68	37850.0/	! fit btw. 500 and 2000 K with MAE of 9.9%, 20.9%		
PLOG/3.000E-02	6.37E+100	-26.54	71530.0/			
PLOG/3.000E-02	3.15E+81	-21.50	53110.0/	! fit btw. 500 and 1300 K with MAE of 6.4%, 18.1%		
PLOG/3.947E-02	1.10E+73	-18.60	52250.0/			
PLOG/3.947E-02	3.29E+49	-12.41	36940.0/	! fit btw. 500 and 1300 K with MAE of 6.6%, 20.2%		
PLOG/1.000E+00	1.33E+52	-11.82	45990.0/			
PLOG/1.000E+00	1.50E+35	-13.00	688.9/	! fit btw. 500 and 1500 K with MAE of 3.2%, 6.5%		
PLOG/1.000E+01	4.96E+82	-20.44	67550.0/			
PLOG/1.000E+01	1.61E+29	-4.91	35890.0/	! fit btw. 500 and 1700 K with MAE of 0.4%, 0.9%		
PLOG/1.000E+02	7.03E+66	-15.40	63890.0/			
PLOG/1.000E+02	8.34E+23	-3.19	34410.0/	! fit btw. 500 and 2000 K with MAE of 0.6%, 1.4%		

C₆H₁₃ (3-hexyl) → C₅H₁₀ (1-pentene) + CH₃				6.93E+29	-4.83	39170.0
PLOG/3.000E-02	2.12E+67	-17.04	49470.0/	! fit btw. 500 and 1300 K with MAE of 6.6%, 20.6%		
PLOG/3.947E-02	5.05E+67	-17.11	49920.0/	! fit btw. 500 and 1300 K with MAE of 7.3%, 23.2%		
PLOG/1.000E+00	1.97E+49	-11.05	45180.0/	! fit btw. 500 and 1500 K with MAE of 5.9%, 14.6%		
PLOG/1.000E+01	1.63E+39	-7.79	42340.0/	! fit btw. 500 and 1700 K with MAE of 8.7%, 19.3%		
PLOG/1.000E+02	6.93E+29	-4.83	39170.0/	! fit btw. 500 and 2000 K with MAE of 10.3%, 22.1%		
PLOG/3.000E-02	2.69E+99	-26.21	71470.0/			
PLOG/3.000E-02	3.52E+82	-21.89	54360.0/	! fit btw. 500 and 1300 K with MAE of 6.3%, 17.8%		
PLOG/3.947E-02	4.86E+73	-18.85	53340.0/			
PLOG/3.947E-02	1.85E+52	-13.22	39380.0/	! fit btw. 500 and 1300 K with MAE of 6.4%, 19.8%		
PLOG/1.000E+00	1.38E+53	-12.16	47380.0/			
PLOG/1.000E+00	4.10E+35	-13.70	-1432.0/	! fit btw. 500 and 1500 K with MAE of 3.5%, 6.7%		
PLOG/1.000E+01	3.48E+83	-20.71	68910.0/			
PLOG/1.000E+01	3.38E+29	-5.03	37060.0/	! fit btw. 500 and 1700 K with MAE of 0.5%, 0.9%		
PLOG/1.000E+02	1.86E+67	-15.53	65130.0/			
PLOG/1.000E+02	1.06E+24	-3.24	35520.0/	! fit btw. 500 and 2000 K with MAE of 0.6%, 1.5%		
C₇H₁₅ (1-heptyl) → C₂H₄ + C₅H₁₁				1.77E+28	-4.33	36730.0
PLOG/3.000E-02	1.66E+12	0.00	28920.0/	! fit btw. 500 and 700 K with MAE of 4.8%, 7.4%		
PLOG/3.947E-02	2.25E-64	23.66	1189.0/	! fit btw. 500 and 800 K with MAE of 9.9%, 17.4%		
PLOG/1.000E+00	9.06E+30	-5.68	34680.0/	! fit btw. 500 and 1100 K with MAE of 2.8%, 4.3%		
PLOG/1.000E+01	1.42E+35	-6.62	38340.0/	! fit btw. 500 and 1400 K with MAE of 3.4%, 7.3%		
PLOG/1.000E+02	1.77E+28	-4.33	36730.0/	! fit btw. 500 and 1800 K with MAE of 7.4%, 14.4%		
PLOG/3.000E-02	1.66E+12	0.00	28920.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 4.8%, 7.4%		
PLOG/3.947E-02	2.25E-64	23.66	1189.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 9.9%, 17.4%		
PLOG/1.000E+00	2.86E+26	-3.48	49000.0/			
PLOG/1.000E+00	6.38E+36	-7.49	36930.0/	! fit btw. 500 and 1100 K with MAE of 0.2%, 0.4%		
PLOG/1.000E+01	9.31E+40	-8.30	41840.0/			
PLOG/1.000E+01	3.89E+28	-5.41	31480.0/	! fit btw. 500 and 1400 K with MAE of 0.6%, 1.1%		
PLOG/1.000E+02	3.23E+59	-13.33	57960.0/			
PLOG/1.000E+02	1.28E+24	-3.21	34030.0/	! fit btw. 500 and 1800 K with MAE of 0.4%, 0.7%		

C₇H₁₅ (1-heptyl) → C₃H₆ + C₄H₉				6.13E+36	-6.91	47810.0
PLOG/3.000E-02	7.97E+13	0.00	31480.0/	! fit btw. 500 and 700 K with MAE of 1.7%, 2.5%		
PLOG/3.947E-02	6.50E-50	19.72	8934.0/	! fit btw. 500 and 800 K with MAE of 10.7%, 19.0%		
PLOG/1.000E+00	5.11E+32	-5.74	40960.0/	! fit btw. 500 and 1100 K with MAE of 3.6%, 8.1%		
PLOG/1.000E+01	1.25E+44	-9.12	48380.0/	! fit btw. 500 and 1400 K with MAE of 16.7%, 30.5%		
PLOG/1.000E+02	6.13E+36	-6.91	47810.0/	! fit btw. 500 and 1800 K with MAE of 25.8%, 56.9%		
PLOG/3.000E-02	7.97E+13	0.00	31480.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 1.7%, 2.5%		
PLOG/3.947E-02	6.50E-50	19.72	8934.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 10.7%, 19.0%		
PLOG/1.000E+00	4.53E+38	-7.51	43890.0/			
PLOG/1.000E+00	1.03E+19	-8.25	-4533.0/	! fit btw. 500 and 1100 K with MAE of 1.8%, 5.2%		
PLOG/1.000E+01	9.19E+93	-23.63	77650.0/			
PLOG/1.000E+01	4.70E+32	-5.98	41450.0/	! fit btw. 500 and 1400 K with MAE of 0.7%, 1.4%		
PLOG/1.000E+02	5.26E+79	-19.12	76790.0/			
PLOG/1.000E+02	1.99E+26	-4.14	40450.0/	! fit btw. 500 and 1800 K with MAE of 2.0%, 4.5%		
C₇H₁₅ (1-heptyl) → C₆H₁₂ (1-hexene) + CH₃				1.00E+38	-7.22	48070.0
PLOG/3.000E-02	5.97E+12	0.00	29120.0/	! fit btw. 500 and 700 K with MAE of 1.6%, 2.4%		
PLOG/3.947E-02	5.62E-47	18.46	7982.0/	! fit btw. 500 and 800 K with MAE of 10.4%, 18.5%		
PLOG/1.000E+00	2.91E+40	-8.22	42830.0/	! fit btw. 500 and 1100 K with MAE of 2.4%, 4.4%		
PLOG/1.000E+01	3.14E+46	-9.84	48840.0/	! fit btw. 500 and 1400 K with MAE of 13.4%, 26.7%		
PLOG/1.000E+02	1.00E+38	-7.22	48070.0/	! fit btw. 500 and 1800 K with MAE of 23.5%, 52.3%		
PLOG/3.000E-02	5.97E+12	0.00	29120.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 1.6%, 2.4%		
PLOG/3.947E-02	5.62E-47	18.46	7982.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 10.4%, 18.5%		
PLOG/1.000E+00	1.49E+43	-9.03	44160.0/			
PLOG/1.000E+00	1.44E+25	-11.19	-8403.0/	! fit btw. 500 and 1100 K with MAE of 1.9%, 4.5%		
PLOG/1.000E+01	1.15E+91	-22.84	74640.0/			
PLOG/1.000E+01	6.69E+33	-6.28	41640.0/	! fit btw. 500 and 1400 K with MAE of 0.4%, 1.0%		
PLOG/1.000E+02	3.42E+78	-18.76	75290.0/			
PLOG/1.000E+02	1.07E+27	-4.29	40640.0/	! fit btw. 500 and 1800 K with MAE of 1.7%, 3.8%		



8.45E+37 -7.20 47410.0

PLOG/3.000E-02	7.00E+12	0.00	28580.0/	! fit btw. 500 and 700 K with MAE of 1.5%, 2.3%
PLOG/3.947E-02	1.95E-46	18.31	7623.0/	! fit btw. 500 and 800 K with MAE of 10.4%, 18.5%
PLOG/1.000E+00	2.70E+40	-8.20	42290.0/	! fit btw. 500 and 1100 K with MAE of 2.4%, 4.4%
PLOG/1.000E+01	2.07E+46	-9.78	48190.0/	! fit btw. 500 and 1400 K with MAE of 13.3%, 26.5%
PLOG/1.000E+02	8.45E+37	-7.20	47410.0/	! fit btw. 500 and 1800 K with MAE of 23.2%, 51.5%

PLOG/3.000E-02	7.00E+12	0.00	28580.0/	
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 1.5%, 2.3%
PLOG/3.947E-02	1.95E-46	18.31	7623.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 10.4%, 18.5%
PLOG/1.000E+00	1.26E+43	-8.99	43600.0/	
PLOG/1.000E+00	1.00E+25	-11.14	-9026.0/	! fit btw. 500 and 1100 K with MAE of 1.9%, 4.5%
PLOG/1.000E+01	5.58E+90	-22.75	73920.0/	
PLOG/1.000E+01	5.73E+33	-6.25	41050.0/	! fit btw. 500 and 1400 K with MAE of 0.4%, 0.9%
PLOG/1.000E+02	1.94E+78	-18.69	74530.0/	
PLOG/1.000E+02	1.24E+27	-4.31	40070.0/	! fit btw. 500 and 1800 K with MAE of 1.6%, 3.7%



1.01E+35 -6.24 49340.0

PLOG/3.000E-02	1.36E+14	0.00	34110.0/	! fit btw. 500 and 700 K with MAE of 5.7%, 8.8%
PLOG/3.947E-02	3.68E-97	34.51	-5757.0/	! fit btw. 500 and 800 K with MAE of 15.8%, 29.2%
PLOG/1.000E+00	5.75E+24	-3.34	39170.0/	! fit btw. 500 and 1100 K with MAE of 3.0%, 6.6%
PLOG/1.000E+01	4.10E+41	-8.31	49210.0/	! fit btw. 500 and 1400 K with MAE of 15.1%, 28.7%
PLOG/1.000E+02	1.01E+35	-6.24	49340.0/	! fit btw. 500 and 1800 K with MAE of 26.4%, 59.2%

PLOG/3.000E-02	1.36E+14	0.00	34110.0/	
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 5.7%, 8.8%
PLOG/3.947E-02	3.68E-97	34.51	-5757.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 15.8%, 29.2%
PLOG/1.000E+00	1.81E+41	-8.33	46500.0/	
PLOG/1.000E+00	5.28E-78	27.17	-4845.0/	! fit btw. 500 and 1100 K with MAE of 1.0%, 1.9%
PLOG/1.000E+01	2.60E+86	-21.35	75470.0/	
PLOG/1.000E+01	1.21E+30	-5.13	42260.0/	! fit btw. 500 and 1400 K with MAE of 0.6%, 1.1%
PLOG/1.000E+02	1.58E+76	-17.95	77140.0/	
PLOG/1.000E+02	2.08E+24	-3.45	41690.0/	! fit btw. 500 and 1800 K with MAE of 2.0%, 4.5%

C₇H₁₅ (1-heptyl) → C₇H₁₄ (1-heptene) + H				7.65E+29	-5.03	43130.0
PLOG/3.000E-02	2.13E+11	0.00	34290.0/	! fit btw. 500 and 700 K with MAE of 1.3%, 1.9%		
PLOG/3.947E-02	7.97E-52	19.50	11700.0/	! fit btw. 500 and 800 K with MAE of 10.7%, 19.1%		
PLOG/1.000E+00	6.42E+30	-5.95	39810.0/	! fit btw. 500 and 1100 K with MAE of 2.5%, 4.0%		
PLOG/1.000E+01	8.93E+37	-7.73	44870.0/	! fit btw. 500 and 1400 K with MAE of 3.6%, 8.0%		
PLOG/1.000E+02	7.65E+29	-5.03	43130.0/	! fit btw. 500 and 1800 K with MAE of 8.6%, 17.1%		
PLOG/3.000E-02	2.13E+11	0.00	34290.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 1.3%, 1.9%		
PLOG/3.947E-02	7.97E-52	19.50	11700.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 10.7%, 19.1%		
PLOG/1.000E+00	5.30E+35	-7.47	41710.0/			
PLOG/1.000E+00	1.55E-10	6.81	34340.0/	! fit btw. 500 and 1100 K with MAE of 0.3%, 0.5%		
PLOG/1.000E+01	6.83E+43	-9.43	48380.0/			
PLOG/1.000E+01	3.64E+31	-6.66	37510.0/	! fit btw. 500 and 1400 K with MAE of 0.7%, 1.3%		
PLOG/1.000E+02	9.04E+62	-14.54	65350.0/			
PLOG/1.000E+02	6.81E+24	-3.65	39920.0/	! fit btw. 500 and 1800 K with MAE of 0.4%, 0.9%		
C₇H₁₅ (2-heptyl) → C₂H₄ + C₅H₁₁				3.48E+38	-7.47	52210.0
PLOG/3.000E-02	6.79E+81	-21.48	58160.0/	! fit btw. 500 and 1000 K with MAE of 2.2%, 4.7%		
PLOG/3.947E-02	3.16E+78	-20.42	57200.0/	! fit btw. 500 and 1000 K with MAE of 3.1%, 6.6%		
PLOG/1.000E+00	1.05E+66	-16.05	57550.0/	! fit btw. 500 and 1300 K with MAE of 8.9%, 21.7%		
PLOG/1.000E+01	3.70E+52	-11.74	55570.0/	! fit btw. 500 and 1500 K with MAE of 17.0%, 32.6%		
PLOG/1.000E+02	3.48E+38	-7.47	52210.0/	! fit btw. 500 and 1900 K with MAE of 28.0%, 62.3%		
PLOG/3.000E-02	6.79E+81	-21.48	58160.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 2.2%, 4.7%		
PLOG/3.947E-02	3.16E+78	-20.42	57200.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 3.1%, 6.6%		
PLOG/1.000E+00	5.16E+75	-18.89	62750.0/			
PLOG/1.000E+00	1.02E+123	-36.72	60820.0/	! fit btw. 500 and 1300 K with MAE of 3.5%, 11.7%		
PLOG/1.000E+01	1.78E+11	-2.64	17500.0/			
PLOG/1.000E+01	4.48E+59	-13.78	59770.0/	! fit btw. 500 and 1500 K with MAE of 9.6%, 26.2%		
PLOG/1.000E+02	1.42E+43	-8.77	55450.0/			
PLOG/1.000E+02	3.99E+24	-5.59	31940.0/	! fit btw. 500 and 1900 K with MAE of 20.3%, 59.9%		

C₇H₁₅ (2-heptyl) → C₃H₆ + C₄H₉				7.66E+28	-4.47	37750.0
PLOG/3.000E-02	7.02E+63	-15.93	46950.0/	! fit btw. 500 and 1000 K with MAE of 1.8%, 3.9%		
PLOG/3.947E-02	4.12E+61	-15.21	46270.0/	! fit btw. 500 and 1000 K with MAE of 1.9%, 3.5%		
PLOG/1.000E+00	5.88E+48	-10.81	43960.0/	! fit btw. 500 and 1300 K with MAE of 5.6%, 13.3%		
PLOG/1.000E+01	2.47E+37	-7.16	40570.0/	! fit btw. 500 and 1500 K with MAE of 8.9%, 16.0%		
PLOG/1.000E+02	7.66E+28	-4.47	37750.0/	! fit btw. 500 and 1900 K with MAE of 9.9%, 19.7%		
PLOG/3.000E-02	7.02E+63	-15.93	46950.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 1.8%, 3.9%		
PLOG/3.947E-02	4.12E+61	-15.21	46270.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 1.9%, 3.5%		
PLOG/1.000E+00	4.69E+12	-1.06	22340.0/			
PLOG/1.000E+00	3.31E+56	-13.08	48190.0/	! fit btw. 500 and 1300 K with MAE of 1.6%, 3.2%		
PLOG/1.000E+01	9.37E+85	-21.33	69530.0/			
PLOG/1.000E+01	1.08E+30	-5.08	36430.0/	! fit btw. 500 and 1500 K with MAE of 0.3%, 0.7%		
PLOG/1.000E+02	1.41E+44	-8.76	49280.0/			
PLOG/1.000E+02	4.47E+30	-5.36	36130.0/	! fit btw. 500 and 1900 K with MAE of 1.4%, 3.0%		
C₇H₁₅ (2-heptyl) → C₆H₁₂ (1-hexene) + CH₃				3.25E+44	-9.10	56690.0
PLOG/3.000E-02	1.88E+86	-22.72	59720.0/	! fit btw. 500 and 1000 K with MAE of 1.8%, 3.6%		
PLOG/3.947E-02	5.31E+83	-21.89	59190.0/	! fit btw. 500 and 1000 K with MAE of 3.1%, 8.0%		
PLOG/1.000E+00	1.83E+76	-18.96	63280.0/	! fit btw. 500 and 1300 K with MAE of 10.9%, 28.8%		
PLOG/1.000E+01	1.44E+59	-13.56	60080.0/	! fit btw. 500 and 1500 K with MAE of 23.3%, 48.0%		
PLOG/1.000E+02	3.25E+44	-9.10	56690.0/	! fit btw. 500 and 1900 K with MAE of 34.5%, 95.4%		
PLOG/3.000E-02	1.88E+86	-22.72	59720.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 1.8%, 3.6%		
PLOG/3.947E-02	5.31E+83	-21.89	59190.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 3.1%, 8.0%		
PLOG/1.000E+00	5.82E+88	-22.63	69990.0/			
PLOG/1.000E+00	3.60E+134	-39.99	67150.0/	! fit btw. 500 and 1300 K with MAE of 3.7%, 10.5%		
PLOG/1.000E+01	-3.88E+64	-15.56	56900.0/			
PLOG/1.000E+01	1.66E+53	-11.97	53020.0/	! fit btw. 500 and 1500 K with MAE of 14.3%, 36.7%		
PLOG/1.000E+02	9.24E+84	-20.51	84980.0/			
PLOG/1.000E+02	9.85E+40	-8.67	50710.0/	! fit btw. 500 and 1900 K with MAE of 5.2%, 21.9%		

C₇H₁₅ (2-heptyl) → C₄H₈ (1-butene) + C₃H₇				3.61E+44	-9.11	56120.0
PLOG/3.000E-02	1.56E+86	-22.66	59290.0/	! fit btw. 500 and 1000 K with MAE of 1.9%, 3.7%		
PLOG/3.947E-02	4.24E+83	-21.82	58740.0/	! fit btw. 500 and 1000 K with MAE of 3.1%, 8.0%		
PLOG/1.000E+00	1.09E+76	-18.88	62710.0/	! fit btw. 500 and 1300 K with MAE of 11.0%, 29.1%		
PLOG/1.000E+01	9.64E+58	-13.50	59460.0/	! fit btw. 500 and 1500 K with MAE of 23.3%, 47.8%		
PLOG/1.000E+02	3.61E+44	-9.11	56120.0/	! fit btw. 500 and 1900 K with MAE of 34.4%, 98.0%		
PLOG/3.000E-02	1.56E+86	-22.66	59290.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 1.9%, 3.7%		
PLOG/3.947E-02	4.24E+83	-21.82	58740.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 3.1%, 8.0%		
PLOG/1.000E+00	5.77E+88	-22.61	69540.0/			
PLOG/1.000E+00	5.65E+143	-42.79	70330.0/	! fit btw. 500 and 1300 K with MAE of 3.7%, 10.7%		
PLOG/1.000E+01	-2.61E+64	-15.51	56250.0/			
PLOG/1.000E+01	1.11E+53	-11.91	52370.0/	! fit btw. 500 and 1500 K with MAE of 14.3%, 36.6%		
PLOG/1.000E+02	1.43E+85	-20.57	84540.0/			
PLOG/1.000E+02	2.23E+41	-8.77	50290.0/	! fit btw. 500 and 1900 K with MAE of 5.4%, 23.3%		
C₇H₁₅ (2-heptyl) → C₅H₁₀ (1-pentene) + C₂H₅				1.67E+56	-12.69	68980.0
PLOG/3.000E-02	4.61E+104	-28.20	69600.0/	! fit btw. 500 and 1000 K with MAE of 3.4%, 7.5%		
PLOG/3.947E-02	5.11E+93	-24.84	65530.0/	! fit btw. 500 and 1000 K with MAE of 13.8%, 42.3%		
PLOG/1.000E+00	4.95E+88	-22.71	72020.0/	! fit btw. 500 and 1300 K with MAE of 19.7%, 56.8%		
PLOG/1.000E+01	8.39E+73	-18.01	71780.0/	! fit btw. 500 and 1500 K with MAE of 33.5%, 74.3%		
PLOG/1.000E+02	1.67E+56	-12.69	68980.0/	! fit btw. 500 and 1900 K with MAE of 55.6%, 158.1%		
PLOG/3.000E-02	4.61E+104	-28.20	69600.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 3.4%, 7.5%		
PLOG/3.947E-02	5.11E+93	-24.84	65530.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 13.8%, 42.3%		
PLOG/1.000E+00	2.29E+100	-26.14	78250.0/			
PLOG/1.000E+00	5.56E+73	-26.04	17690.0/	! fit btw. 500 and 1300 K with MAE of 13.8%, 63.5%		
PLOG/1.000E+01	-3.91E+79	-20.07	68730.0/			
PLOG/1.000E+01	9.14E+67	-16.41	64720.0/	! fit btw. 500 and 1500 K with MAE of 21.9%, 86.0%		
PLOG/1.000E+02	2.96E+85	-20.98	88530.0/			
PLOG/1.000E+02	4.05E+130	-37.28	86560.0/	! fit btw. 500 and 1900 K with MAE of 26.1%, 98.2%		

C₇H₁₅ (3-heptyl) → C₂H₄ + C₅H₁₁				1.39E+36	-6.65	49640.0
PLOG/3.000E-02	5.08E+68	-17.57	51090.0/	! fit btw. 500 and 1100 K with MAE of 4.5%, 6.3%		
PLOG/3.947E-02	1.75E+51	-12.28	43700.0/	! fit btw. 500 and 1100 K with MAE of 28.8%, 104.0%		
PLOG/1.000E+00	2.51E+58	-13.75	52240.0/	! fit btw. 500 and 1300 K with MAE of 8.7%, 29.1%		
PLOG/1.000E+01	7.80E+49	-10.85	52780.0/	! fit btw. 500 and 1600 K with MAE of 16.7%, 40.2%		
PLOG/1.000E+02	1.39E+36	-6.65	49640.0/	! fit btw. 500 and 1900 K with MAE of 31.2%, 88.0%		
PLOG/3.000E-02	4.03E+89	-23.70	63190.0/			
PLOG/3.000E-02	2.54E+72	-19.05	50550.0/	! fit btw. 500 and 1100 K with MAE of 1.9%, 3.8%		
PLOG/3.947E-02	4.38E+50	-11.82	51230.0/			
PLOG/3.947E-02	1.22E+54	-13.18	44630.0/	! fit btw. 500 and 1100 K with MAE of 29.1%, 100.6%		
PLOG/1.000E+00	5.10E+57	-12.10	82090.0/			
PLOG/1.000E+00	9.26E+61	-14.84	53680.0/	! fit btw. 500 and 1300 K with MAE of 7.4%, 21.5%		
PLOG/1.000E+01	1.35E+55	-12.37	55880.0/			
PLOG/1.000E+01	8.47E+35	-13.65	4210.0/	! fit btw. 500 and 1600 K with MAE of 12.3%, 39.7%		
PLOG/1.000E+02	3.65E+40	-7.91	52600.0/			
PLOG/1.000E+02	1.74E+10	-1.51	22390.0/	! fit btw. 500 and 1900 K with MAE of 24.6%, 81.9%		
C₇H₁₅ (3-heptyl) → C₃H₆ + C₄H₉				6.51E+41	-8.23	54350.0
PLOG/3.000E-02	8.84E+74	-19.14	54390.0/	! fit btw. 500 and 1100 K with MAE of 6.0%, 14.3%		
PLOG/3.947E-02	9.05E+33	-6.77	36880.0/	! fit btw. 500 and 1100 K with MAE of 92.0%, 454.1%		
PLOG/1.000E+00	6.55E+72	-17.86	60690.0/	! fit btw. 500 and 1300 K with MAE of 15.0%, 46.8%		
PLOG/1.000E+01	1.71E+46	-9.61	53250.0/	! fit btw. 500 and 1600 K with MAE of 33.5%, 81.8%		
PLOG/1.000E+02	6.51E+41	-8.23	54350.0/	! fit btw. 500 and 1900 K with MAE of 29.7%, 74.6%		
PLOG/3.000E-02	2.93E+81	-21.14	56980.0/			
PLOG/3.000E-02	1.47E+83	-10.15	236100.0/	! fit btw. 500 and 1100 K with MAE of 2.4%, 7.5%		
PLOG/3.947E-02	1.45E+33	-5.77	49800.0/			
PLOG/3.947E-02	7.22E+36	-7.73	37500.0/	! fit btw. 500 and 1100 K with MAE of 88.2%, 401.7%		
PLOG/1.000E+00	2.83E+80	-20.10	64770.0/			
PLOG/1.000E+00	2.67E+57	-21.45	4072.0/	! fit btw. 500 and 1300 K with MAE of 11.7%, 50.2%		
PLOG/1.000E+01	4.03E+52	-11.45	57020.0/			
PLOG/1.000E+01	2.95E+30	-13.14	-4069.0/	! fit btw. 500 and 1600 K with MAE of 27.8%, 74.5%		
PLOG/1.000E+02	2.08E+89	-21.73	86500.0/			
PLOG/1.000E+02	7.76E+25	-3.86	44380.0/	! fit btw. 500 and 1900 K with MAE of 2.3%, 6.0%		

C₇H₁₅ (3-heptyl) → C₆H₁₂ (1-hexene) + CH₃				1.71E+29	-4.65	38890.0
PLOG/3.000E-02	1.18E+66	-16.72	48740.0/	! fit btw. 500 and 1100 K with MAE of 5.4%, 7.4%		
PLOG/3.947E-02	1.71E+51	-12.22	42460.0/	! fit btw. 500 and 1100 K with MAE of 23.7%, 80.3%		
PLOG/1.000E+00	1.27E+48	-10.73	44430.0/	! fit btw. 500 and 1300 K with MAE of 5.9%, 12.7%		
PLOG/1.000E+01	2.95E+42	-8.77	43730.0/	! fit btw. 500 and 1600 K with MAE of 15.5%, 47.0%		
PLOG/1.000E+02	1.71E+29	-4.65	38890.0/	! fit btw. 500 and 1900 K with MAE of 11.1%, 24.1%		
PLOG/3.000E-02	2.56E+98	-26.18	67450.0/			
PLOG/3.000E-02	9.18E+74	-19.75	50380.0/	! fit btw. 500 and 1100 K with MAE of 1.9%, 2.9%		
PLOG/3.947E-02	4.19E+50	-11.87	48310.0/			
PLOG/3.947E-02	8.16E+53	-13.07	43330.0/	! fit btw. 500 and 1100 K with MAE of 23.8%, 78.8%		
PLOG/1.000E+00	3.28E+53	-12.31	47320.0/			
PLOG/1.000E+00	2.25E+37	-11.71	14850.0/	! fit btw. 500 and 1300 K with MAE of 3.0%, 10.9%		
PLOG/1.000E+01	1.43E+76	-18.36	66530.0/			
PLOG/1.000E+01	6.06E+48	-11.05	43920.0/	! fit btw. 500 and 1600 K with MAE of 5.2%, 17.0%		
PLOG/1.000E+02	8.57E+33	-6.03	41330.0/			
PLOG/1.000E+02	2.63E+23	-4.27	86010.0/	! fit btw. 500 and 1900 K with MAE of 13.7%, 32.4%		
C₇H₁₅ (3-heptyl) → C₄H₈ (1-butene) + C₃H₇				1.12E+29	-4.60	38080.0
PLOG/3.000E-02	2.95E+65	-16.51	47960.0/	! fit btw. 500 and 1100 K with MAE of 5.6%, 7.7%		
PLOG/3.947E-02	1.72E+51	-12.19	41930.0/	! fit btw. 500 and 1100 K with MAE of 22.7%, 75.7%		
PLOG/1.000E+00	3.19E+47	-10.54	43540.0/	! fit btw. 500 and 1300 K with MAE of 5.7%, 12.3%		
PLOG/1.000E+01	1.22E+42	-8.66	42880.0/	! fit btw. 500 and 1600 K with MAE of 15.4%, 47.0%		
PLOG/1.000E+02	1.12E+29	-4.60	38080.0/	! fit btw. 500 and 1900 K with MAE of 10.7%, 23.6%		
PLOG/3.000E-02	4.43E+99	-26.50	67710.0/			
PLOG/3.000E-02	1.46E+75	-19.79	49910.0/	! fit btw. 500 and 1100 K with MAE of 1.8%, 2.8%		
PLOG/3.947E-02	4.36E+50	-11.87	47430.0/			
PLOG/3.947E-02	7.39E+53	-13.03	42780.0/	! fit btw. 500 and 1100 K with MAE of 22.8%, 74.4%		
PLOG/1.000E+00	7.23E+52	-12.11	46410.0/			
PLOG/1.000E+00	1.97E+37	-11.21	17130.0/	! fit btw. 500 and 1300 K with MAE of 2.9%, 10.6%		
PLOG/1.000E+01	1.67E+76	-18.37	66050.0/			
PLOG/1.000E+01	3.55E+48	-10.97	43200.0/	! fit btw. 500 and 1600 K with MAE of 5.2%, 17.1%		
PLOG/1.000E+02	1.30E+48	-9.95	52600.0/			
PLOG/1.000E+02	5.21E+32	-6.03	37450.0/	! fit btw. 500 and 1900 K with MAE of 1.2%, 4.5%		

C₇H₁₅ (3-heptyl) → C₅H₁₀ (1-pentene) + C₂H₅				6.01E+58	-13.38	68550.0
PLOG/3.000E-02	9.91E+91	-24.38	63190.0/	! fit btw. 500 and 1100 K with MAE of 7.3%, 11.1%		
PLOG/3.947E-02	3.36E+90	-23.88	63110.0/	! fit btw. 500 and 1100 K with MAE of 6.7%, 10.0%		
PLOG/1.000E+00	5.77E+74	-18.47	64360.0/	! fit btw. 500 and 1300 K with MAE of 13.2%, 40.3%		
PLOG/1.000E+01	9.84E+68	-16.49	67770.0/	! fit btw. 500 and 1600 K with MAE of 51.0%, 250.5%		
PLOG/1.000E+02	6.01E+58	-13.38	68550.0/	! fit btw. 500 and 1900 K with MAE of 85.2%, 484.1%		
PLOG/3.000E-02	1.15E+132	-36.12	85820.0/			
PLOG/3.000E-02	2.26E+103	-28.21	65480.0/	! fit btw. 500 and 1100 K with MAE of 2.7%, 6.4%		
PLOG/3.947E-02	3.36E+90	-23.88	63110.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1100 K with MAE of 6.7%, 10.0%		
PLOG/1.000E+00	4.00E+33	-22.03	-50420.0/			
PLOG/1.000E+00	5.53E+78	-19.64	66490.0/	! fit btw. 500 and 1300 K with MAE of 11.8%, 44.6%		
PLOG/1.000E+01	5.52E+77	-19.01	72950.0/			
PLOG/1.000E+01	2.77E+52	-19.83	9465.0/	! fit btw. 500 and 1600 K with MAE of 44.5%, 249.3%		
PLOG/1.000E+02	8.06E+63	-14.81	72400.0/			
PLOG/1.000E+02	2.56E+32	-11.42	19830.0/	! fit btw. 500 and 1900 K with MAE of 73.1%, 495.1%		
C₇H₁₅ (4-heptyl) → C₂H₄ + C₅H₁₁				1.65E+37	-6.94	53920.0
PLOG/3.000E-02	2.91E+83	-21.99	60410.0/	! fit btw. 500 and 1100 K with MAE of 4.2%, 6.1%		
PLOG/3.947E-02	8.01E+62	-15.67	52410.0/	! fit btw. 500 and 1200 K with MAE of 20.9%, 47.7%		
PLOG/1.000E+00	1.58E+54	-12.48	53920.0/	! fit btw. 500 and 1400 K with MAE of 19.5%, 46.7%		
PLOG/1.000E+01	2.50E+50	-11.01	56480.0/	! fit btw. 500 and 1600 K with MAE of 16.2%, 35.3%		
PLOG/1.000E+02	1.65E+37	-6.94	53920.0/	! fit btw. 500 and 1900 K with MAE of 29.7%, 67.2%		
PLOG/3.000E-02	5.95E+121	-33.62	77380.0/			
PLOG/3.000E-02	2.02E+33	-6.97	38770.0/	! fit btw. 500 and 1100 K with MAE of 0.3%, 0.6%		
PLOG/3.947E-02	1.38E+83	-21.85	60670.0/			
PLOG/3.947E-02	3.65E+61	-11.07	122500.0/	! fit btw. 500 and 1200 K with MAE of 2.4%, 7.3%		
PLOG/1.000E+00	1.44E+65	-15.79	58630.0/			
PLOG/1.000E+00	1.03E+59	-4.96	235900.0/	! fit btw. 500 and 1400 K with MAE of 7.6%, 20.3%		
PLOG/1.000E+01	5.52E+57	-13.13	60840.0/			
PLOG/1.000E+01	4.97E+19	-18.29	-58370.0/	! fit btw. 500 and 1600 K with MAE of 11.1%, 34.9%		
PLOG/1.000E+02	1.56E+52	-11.19	63890.0/			
PLOG/1.000E+02	3.13E+175	-51.53	94610.0/	! fit btw. 500 and 1900 K with MAE of 15.4%, 50.6%		

C₇H₁₅ (4-heptyl) → C₃H₆ + C₄H₉				1.91E+57	-12.96	70020.0
PLOG/3.000E-02	1.04E+104	-28.01	69410.0/	! fit btw. 500 and 1100 K with MAE of 3.1%, 7.5%		
PLOG/3.947E-02	3.60E+65	-16.21	54300.0/	! fit btw. 500 and 1200 K with MAE of 43.6%, 138.8%		
PLOG/1.000E+00	1.08E+54	-12.21	57350.0/	! fit btw. 500 and 1400 K with MAE of 66.3%, 216.8%		
PLOG/1.000E+01	4.21E+74	-18.19	72430.0/	! fit btw. 500 and 1500 K with MAE of 29.5%, 66.3%		
PLOG/1.000E+02	1.91E+57	-12.96	70020.0/	! fit btw. 500 and 1900 K with MAE of 45.2%, 131.9%		
PLOG/3.000E-02	3.78E+108	-29.36	71650.0/			
PLOG/3.000E-02	9.21E+88	-31.37	15810.0/	! fit btw. 500 and 1100 K with MAE of 2.2%, 4.1%		
PLOG/3.947E-02	1.10E+103	-27.66	69640.0/			
PLOG/3.947E-02	7.60E+75	-5.85	284200.0/	! fit btw. 500 and 1200 K with MAE of 3.2%, 7.1%		
PLOG/1.000E+00	1.17E+90	-23.11	72860.0/			
PLOG/1.000E+00	1.82E+60	-3.77	262600.0/	! fit btw. 500 and 1400 K with MAE of 15.1%, 37.2%		
PLOG/1.000E+01	5.10E+82	-20.51	77510.0/			
PLOG/1.000E+01	1.63E+50	-31.81	-67620.0/	! fit btw. 500 and 1500 K with MAE of 16.8%, 49.4%		
PLOG/1.000E+02	4.73E+30	-5.50	54420.0/			
PLOG/1.000E+02	2.17E+124	-32.05	114400.0/	! fit btw. 500 and 1900 K with MAE of 5.5%, 13.2%		
C₇H₁₅ (4-heptyl) → C₆H₁₂ (1-hexene) + CH₃				1.09E+55	-12.24	68710.0
PLOG/3.000E-02	9.22E+90	-24.17	63620.0/	! fit btw. 500 and 1100 K with MAE of 4.6%, 7.6%		
PLOG/3.947E-02	4.50E+63	-15.78	53020.0/	! fit btw. 500 and 1200 K with MAE of 29.8%, 71.2%		
PLOG/1.000E+00	2.72E+59	-13.91	58880.0/	! fit btw. 500 and 1400 K with MAE of 47.5%, 150.0%		
PLOG/1.000E+01	9.77E+89	-22.83	78500.0/	! fit btw. 500 and 1600 K with MAE of 367.7%, 3897.0%		
PLOG/1.000E+02	1.09E+55	-12.24	68710.0/	! fit btw. 500 and 1800 K with MAE of 43.9%, 116.5%		
PLOG/3.000E-02	2.89E+94	-25.24	65010.0/			
PLOG/3.000E-02	4.68E+98	-15.40	240700.0/	! fit btw. 500 and 1100 K with MAE of 2.7%, 7.0%		
PLOG/3.947E-02	2.86E+92	-24.57	64760.0/			
PLOG/3.947E-02	1.11E+62	-11.07	122700.0/	! fit btw. 500 and 1200 K with MAE of 2.2%, 6.7%		
PLOG/1.000E+00	4.45E+86	-22.14	70600.0/			
PLOG/1.000E+00	3.34E+73	-1.91	387400.0/	! fit btw. 500 and 1400 K with MAE of 10.8%, 30.1%		
PLOG/1.000E+01	5.96E+97	-25.05	83630.0/			
PLOG/1.000E+01	4.50E+66	-31.40	-28050.0/	! fit btw. 500 and 1600 K with MAE of 357.5%, 3964.9%		
PLOG/1.000E+02	8.07E+33	-6.47	55270.0/			
PLOG/1.000E+02	1.16E+113	-28.75	107100.0/	! fit btw. 500 and 1800 K with MAE of 3.9%, 10.0%		



1.52E+55 -12.28 68250.0

PLOG/3.000E-02	8.18E+90	-24.12	63240.0/	! fit btw. 500 and 1100 K with MAE of 4.6%, 7.7%
PLOG/3.947E-02	1.71E+63	-15.61	52470.0/	! fit btw. 500 and 1200 K with MAE of 30.2%, 72.4%
PLOG/1.000E+00	1.44E+59	-13.81	58340.0/	! fit btw. 500 and 1400 K with MAE of 48.3%, 153.6%
PLOG/1.000E+01	4.80E+64	-15.18	67070.0/	! fit btw. 500 and 1600 K with MAE of 31.8%, 83.3%
PLOG/1.000E+02	1.52E+55	-12.28	68250.0/	! fit btw. 500 and 1800 K with MAE of 43.8%, 116.1%

PLOG/3.000E-02	2.63E+94	-25.19	64630.0/	
PLOG/3.000E-02	4.98E+98	-15.28	241800.0/	! fit btw. 500 and 1100 K with MAE of 2.8%, 7.1%
PLOG/3.947E-02	2.37E+92	-24.52	64360.0/	
PLOG/3.947E-02	4.32E+61	-10.89	122400.0/	! fit btw. 500 and 1200 K with MAE of 2.3%, 6.4%
PLOG/1.000E+00	6.09E+86	-22.16	70240.0/	
PLOG/1.000E+00	2.48E+73	-1.73	389400.0/	! fit btw. 500 and 1400 K with MAE of 10.9%, 30.4%
PLOG/1.000E+01	1.86E+72	-17.37	71630.0/	
PLOG/1.000E+01	2.56E+31	-20.37	-40870.0/	! fit btw. 500 and 1600 K with MAE of 24.4%, 82.7%
PLOG/1.000E+02	1.19E+34	-6.51	54840.0/	
PLOG/1.000E+02	1.47E+113	-28.78	106600.0/	! fit btw. 500 and 1800 K with MAE of 3.9%, 9.9%



3.65E+27 -4.09 36940.0

PLOG/3.000E-02	2.04E+65	-16.29	47840.0/	! fit btw. 500 and 1100 K with MAE of 2.7%, 4.3%
PLOG/3.947E-02	4.58E+78	-20.33	53580.0/	! fit btw. 500 and 1200 K with MAE of 15.9%, 43.1%
PLOG/1.000E+00	5.51E+58	-13.81	48340.0/	! fit btw. 500 and 1400 K with MAE of 22.5%, 74.1%
PLOG/1.000E+01	6.01E+36	-6.98	40190.0/	! fit btw. 500 and 1600 K with MAE of 9.5%, 18.7%
PLOG/1.000E+02	3.65E+27	-4.09	36940.0/	! fit btw. 500 and 1900 K with MAE of 10.0%, 19.0%

PLOG/3.000E-02	3.51E+97	-26.10	62160.0/	
PLOG/3.000E-02	3.19E+27	-4.99	31510.0/	! fit btw. 500 and 1100 K with MAE of 0.1%, 0.3%
PLOG/3.947E-02	1.29E+84	-21.92	56560.0/	
PLOG/3.947E-02	1.29E+50	-15.32	20030.0/	! fit btw. 500 and 1200 K with MAE of 11.2%, 41.6%
PLOG/1.000E+00	3.68E+124	-32.74	89620.0/	
PLOG/1.000E+00	2.71E+68	-17.09	50080.0/	! fit btw. 500 and 1400 K with MAE of 11.8%, 30.2%
PLOG/1.000E+01	1.24E+86	-21.33	70150.0/	
PLOG/1.000E+01	1.02E+29	-4.78	35840.0/	! fit btw. 500 and 1600 K with MAE of 0.4%, 1.0%
PLOG/1.000E+02	1.94E+63	-14.29	62180.0/	
PLOG/1.000E+02	3.22E+23	-3.02	34130.0/	! fit btw. 500 and 1900 K with MAE of 0.7%, 1.6%

C₈H₁₇ (1-octyl) → C₂H₄ + C₆H₁₃				2.29E+26	-3.78	36080.0
PLOG/3.000E-02	7.45E+11	0.00	28290.0/	! fit btw. 500 and 700 K with MAE of 8.8%, 13.9%		
PLOG/3.947E-02	4.61E+11	0.00	27570.0/	! fit btw. 500 and 700 K with MAE of 6.4%, 10.0%		
PLOG/1.000E+00	1.54E+32	-6.07	35320.0/	! fit btw. 500 and 1100 K with MAE of 3.2%, 5.1%		
PLOG/1.000E+01	2.15E+33	-6.07	37830.0/	! fit btw. 500 and 1400 K with MAE of 3.7%, 7.4%		
PLOG/1.000E+02	2.29E+26	-3.78	36080.0/	! fit btw. 500 and 1800 K with MAE of 7.6%, 13.9%		
PLOG/3.000E-02	7.45E+11	0.00	28290.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 8.8%, 13.9%		
PLOG/3.947E-02	4.61E+11	0.00	27570.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 6.4%, 10.0%		
PLOG/1.000E+00	4.58E+38	-8.07	37820.0/			
PLOG/1.000E+00	3.70E+27	-3.71	51210.0/	! fit btw. 500 and 1100 K with MAE of 0.1%, 0.2%		
PLOG/1.000E+01	1.18E+64	-15.17	55510.0/			
PLOG/1.000E+01	6.58E+27	-4.51	34830.0/	! fit btw. 500 and 1400 K with MAE of 0.1%, 0.2%		
PLOG/1.000E+02	1.47E+54	-11.74	55750.0/			
PLOG/1.000E+02	3.38E+23	-3.07	33890.0/	! fit btw. 500 and 1800 K with MAE of 0.4%, 0.8%		
C₈H₁₇ (1-octyl) → C₃H₆ + C₅H₁₁				2.17E+35	-6.48	49480.0
PLOG/3.000E-02	2.88E+14	0.00	33520.0/	! fit btw. 500 and 700 K with MAE of 6.3%, 9.8%		
PLOG/3.947E-02	2.27E+14	0.00	33390.0/	! fit btw. 500 and 700 K with MAE of 3.7%, 5.7%		
PLOG/1.000E+00	4.50E+34	-6.15	44580.0/	! fit btw. 500 and 1100 K with MAE of 5.4%, 10.3%		
PLOG/1.000E+01	1.17E+46	-9.62	52070.0/	! fit btw. 500 and 1400 K with MAE of 23.1%, 44.4%		
PLOG/1.000E+02	2.17E+35	-6.48	49480.0/	! fit btw. 500 and 1800 K with MAE of 32.1%, 71.6%		
PLOG/3.000E-02	2.88E+14	0.00	33520.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 6.3%, 9.8%		
PLOG/3.947E-02	2.27E+14	0.00	33390.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 3.7%, 5.7%		
PLOG/1.000E+00	2.74E+38	-7.28	46440.0/			
PLOG/1.000E+00	4.70E+18	-9.70	-12080.0/	! fit btw. 500 and 1100 K with MAE of 4.7%, 10.7%		
PLOG/1.000E+01	1.28E+105	-26.79	86390.0/			
PLOG/1.000E+01	1.00E+30	-5.15	42610.0/	! fit btw. 500 and 1400 K with MAE of 0.9%, 1.9%		
PLOG/1.000E+02	-4.68E+77	-19.28	66800.0/			
PLOG/1.000E+02	1.09E+49	-10.53	54650.0/	! fit btw. 500 and 1800 K with MAE of 8.4%, 15.4%		

C₈H₁₇ (1-octyl) → C₇H₁₄ (1-heptene) + CH₃				2.89E+35	-6.56	48540.0
PLOG/3.000E-02	1.29E+14	0.00	33880.0/	! fit btw. 500 and 700 K with MAE of 7.9%, 12.4%		
PLOG/3.947E-02	8.92E+13	0.00	33580.0/	! fit btw. 500 and 700 K with MAE of 5.9%, 9.1%		
PLOG/1.000E+00	3.03E+21	-2.39	37560.0/	! fit btw. 500 and 1100 K with MAE of 4.1%, 9.8%		
PLOG/1.000E+01	5.42E+42	-8.77	49000.0/	! fit btw. 500 and 1400 K with MAE of 15.8%, 28.4%		
PLOG/1.000E+02	2.89E+35	-6.56	48540.0/	! fit btw. 500 and 1800 K with MAE of 25.4%, 54.8%		
PLOG/3.000E-02	1.29E+14	0.00	33880.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 7.9%, 12.4%		
PLOG/3.947E-02	8.92E+13	0.00	33580.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 5.9%, 9.1%		
PLOG/1.000E+00	6.76E+25	-3.72	39290.0/			
PLOG/1.000E+00	6.74E+29	6.68	222000.0/	! fit btw. 500 and 1100 K with MAE of 1.8%, 4.3%		
PLOG/1.000E+01	3.15E+75	-18.25	68730.0/			
PLOG/1.000E+01	4.08E+44	-9.92	46040.0/	! fit btw. 500 and 1400 K with MAE of 0.9%, 1.9%		
PLOG/1.000E+02	1.12E+72	-16.93	73610.0/			
PLOG/1.000E+02	1.54E+30	-5.44	42920.0/	! fit btw. 500 and 1800 K with MAE of 2.3%, 4.4%		
C₈H₁₇ (1-octyl) → C₄H₈ (1-butene) + C₄H₉				2.08E+35	-6.54	47690.0
PLOG/3.000E-02	1.33E+14	0.00	33210.0/	! fit btw. 500 and 700 K with MAE of 8.3%, 13.1%		
PLOG/3.947E-02	9.01E+13	0.00	32900.0/	! fit btw. 500 and 700 K with MAE of 6.3%, 9.8%		
PLOG/1.000E+00	1.32E+21	-2.28	36720.0/	! fit btw. 500 and 1100 K with MAE of 4.1%, 9.8%		
PLOG/1.000E+01	2.70E+42	-8.70	48140.0/	! fit btw. 500 and 1400 K with MAE of 15.6%, 28.0%		
PLOG/1.000E+02	2.08E+35	-6.54	47690.0/	! fit btw. 500 and 1800 K with MAE of 25.1%, 53.8%		
PLOG/3.000E-02	1.33E+14	0.00	33210.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 8.3%, 13.1%		
PLOG/3.947E-02	9.01E+13	0.00	32900.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 6.3%, 9.8%		
PLOG/1.000E+00	3.84E+25	-3.65	38500.0/			
PLOG/1.000E+00	2.16E+29	6.69	218900.0/	! fit btw. 500 and 1100 K with MAE of 1.6%, 4.1%		
PLOG/1.000E+01	2.25E+87	-21.75	74750.0/			
PLOG/1.000E+01	7.79E+32	-6.13	41960.0/	! fit btw. 500 and 1400 K with MAE of 0.7%, 1.4%		
PLOG/1.000E+02	6.51E+75	-18.04	75250.0/			
PLOG/1.000E+02	6.36E+26	-4.38	41130.0/	! fit btw. 500 and 1800 K with MAE of 2.1%, 4.5%		



7.99E+37 -7.14 47410.0

PLOG/3.000E-02	1.47E+13	0.00	28630.0/	! fit btw. 500 and 700 K with MAE of 2.9%, 4.4%
PLOG/3.947E-02	1.39E+13	0.00	28580.0/	! fit btw. 500 and 700 K with MAE of 0.6%, 0.9%
PLOG/1.000E+00	1.58E+43	-8.96	43550.0/	! fit btw. 500 and 1100 K with MAE of 3.0%, 5.3%
PLOG/1.000E+01	5.74E+47	-10.15	48910.0/	! fit btw. 500 and 1400 K with MAE of 14.4%, 28.8%
PLOG/1.000E+02	7.99E+37	-7.14	47410.0/	! fit btw. 500 and 1800 K with MAE of 23.5%, 52.0%

PLOG/3.000E-02	1.47E+13	0.00	28630.0/	
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 2.9%, 4.4%
PLOG/3.947E-02	1.39E+13	0.00	28580.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 0.6%, 0.9%
PLOG/1.000E+00	1.58E+46	-9.85	45030.0/	
PLOG/1.000E+00	1.15E+28	-12.23	-9261.0/	! fit btw. 500 and 1100 K with MAE of 2.4%, 5.5%
PLOG/1.000E+01	9.43E+94	-23.93	76150.0/	
PLOG/1.000E+01	1.49E+34	-6.32	41270.0/	! fit btw. 500 and 1400 K with MAE of 0.4%, 0.9%
PLOG/1.000E+02	6.95E+78	-18.80	74910.0/	
PLOG/1.000E+02	1.04E+27	-4.24	40050.0/	! fit btw. 500 and 1800 K with MAE of 1.7%, 3.9%



9.77E+37 -7.19 47760.0

PLOG/3.000E-02	1.21E+13	0.00	28900.0/	! fit btw. 500 and 700 K with MAE of 2.9%, 4.5%
PLOG/3.947E-02	1.14E+13	0.00	28840.0/	! fit btw. 500 and 700 K with MAE of 0.6%, 0.9%
PLOG/1.000E+00	2.03E+43	-9.02	43870.0/	! fit btw. 500 and 1100 K with MAE of 3.0%, 5.3%
PLOG/1.000E+01	8.07E+47	-10.22	49260.0/	! fit btw. 500 and 1400 K with MAE of 14.4%, 28.9%
PLOG/1.000E+02	9.77E+37	-7.19	47760.0/	! fit btw. 500 and 1800 K with MAE of 23.6%, 52.3%

PLOG/3.000E-02	1.21E+13	0.00	28900.0/	
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 2.9%, 4.5%
PLOG/3.947E-02	1.14E+13	0.00	28840.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 0.6%, 0.9%
PLOG/1.000E+00	1.95E+46	-9.90	45340.0/	
PLOG/1.000E+00	1.41E+28	-12.29	-8979.0/	! fit btw. 500 and 1100 K with MAE of 2.4%, 5.6%
PLOG/1.000E+01	1.57E+95	-24.02	76540.0/	
PLOG/1.000E+01	1.89E+34	-6.38	41600.0/	! fit btw. 500 and 1400 K with MAE of 0.4%, 1.0%
PLOG/1.000E+02	1.04E+79	-18.87	75320.0/	
PLOG/1.000E+02	1.11E+27	-4.26	40360.0/	! fit btw. 500 and 1800 K with MAE of 1.7%, 3.9%

C₈H₁₇ (1-octyl) → C₈H₁₆ (1-octene) + H

5.81E+27 -4.34 42340.0

PLOG/3.000E-02	2.58E+11	0.00	34350.0/	! fit btw. 500 and 700 K with MAE of 6.0%, 9.3%
PLOG/3.947E-02	1.68E+11	0.00	33710.0/	! fit btw. 500 and 700 K with MAE of 4.3%, 6.6%
PLOG/1.000E+00	3.22E+32	-6.42	40510.0/	! fit btw. 500 and 1100 K with MAE of 3.5%, 5.5%
PLOG/1.000E+01	1.20E+36	-7.09	44340.0/	! fit btw. 500 and 1400 K with MAE of 4.1%, 8.4%
PLOG/1.000E+02	5.81E+27	-4.34	42340.0/	! fit btw. 500 and 1800 K with MAE of 9.0%, 16.7%

PLOG/3.000E-02	2.58E+11	0.00	34350.0/	
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 6.0%, 9.3%
PLOG/3.947E-02	1.68E+11	0.00	33710.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 700 K with MAE of 4.3%, 6.6%
PLOG/1.000E+00	2.33E+39	-8.54	43160.0/	
PLOG/1.000E+00	2.89E+09	1.30	45550.0/	! fit btw. 500 and 1100 K with MAE of 0.2%, 0.3%
PLOG/1.000E+01	2.05E+69	-16.92	63290.0/	
PLOG/1.000E+01	8.14E+29	-5.33	41030.0/	! fit btw. 500 and 1400 K with MAE of 0.2%, 0.3%
PLOG/1.000E+02	3.97E+57	-12.88	63210.0/	
PLOG/1.000E+02	1.72E+24	-3.44	39720.0/	! fit btw. 500 and 1800 K with MAE of 0.5%, 1.0%

C₈H₁₇ (2-octyl) → C₂H₄ + C₆H₁₃

9.32E+39 -7.93 55430.0

PLOG/3.000E-02	2.63E+97	-26.36	64850.0/	! fit btw. 500 and 800 K with MAE of 4.6%, 7.3%
PLOG/3.947E-02	1.23E+88	-23.39	61970.0/	! fit btw. 500 and 800 K with MAE of 3.7%, 5.9%
PLOG/1.000E+00	5.39E+72	-17.99	62980.0/	! fit btw. 500 and 1100 K with MAE of 11.0%, 23.4%
PLOG/1.000E+01	1.08E+56	-12.73	60050.0/	! fit btw. 500 and 1400 K with MAE of 24.7%, 48.2%
PLOG/1.000E+02	9.32E+39	-7.93	55430.0/	! fit btw. 500 and 1800 K with MAE of 32.4%, 72.6%

PLOG/3.000E-02	2.63E+97	-26.36	64850.0/	
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 4.6%, 7.3%
PLOG/3.947E-02	1.23E+88	-23.39	61970.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 3.7%, 5.9%
PLOG/1.000E+00	2.07E+104	-27.33	79290.0/	
PLOG/1.000E+00	1.34E+68	-17.46	55810.0/	! fit btw. 500 and 1100 K with MAE of 1.0%, 2.2%
PLOG/1.000E+01	1.89E+119	-31.13	96660.0/	
PLOG/1.000E+01	1.73E+38	-7.74	49810.0/	! fit btw. 500 and 1400 K with MAE of 1.1%, 2.5%
PLOG/1.000E+02	4.34E+74	-17.77	78760.0/	
PLOG/1.000E+02	1.45E+62	-15.62	58200.0/	! fit btw. 500 and 1800 K with MAE of 4.8%, 10.0%

C₈H₁₇ (2-octyl) → C₃H₆ + C₅H₁₁				1.26E+28	-4.24	37240.0
PLOG/3.000E-02	7.89E+62	-15.71	46580.0/	! fit btw. 500 and 800 K with MAE of 3.6%, 5.7%		
PLOG/3.947E-02	1.61E+55	-13.28	43880.0/	! fit btw. 500 and 800 K with MAE of 2.9%, 4.7%		
PLOG/1.000E+00	9.21E+43	-9.44	41340.0/	! fit btw. 500 and 1100 K with MAE of 4.3%, 7.5%		
PLOG/1.000E+01	9.29E+35	-6.76	39610.0/	! fit btw. 500 and 1400 K with MAE of 7.1%, 11.8%		
PLOG/1.000E+02	1.26E+28	-4.24	37240.0/	! fit btw. 500 and 1800 K with MAE of 9.2%, 17.1%		
PLOG/3.000E-02	7.89E+62	-15.71	46580.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 3.6%, 5.7%		
PLOG/3.947E-02	1.61E+55	-13.28	43880.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 2.9%, 4.7%		
PLOG/1.000E+00	9.48E+67	-16.49	54990.0/			
PLOG/1.000E+00	3.33E+47	-10.89	40630.0/	! fit btw. 500 and 1100 K with MAE of 0.3%, 0.7%		
PLOG/1.000E+01	4.12E+78	-19.24	64800.0/			
PLOG/1.000E+01	2.17E+30	-5.19	36310.0/	! fit btw. 500 and 1400 K with MAE of 0.3%, 0.5%		
PLOG/1.000E+02	6.79E+61	-13.89	60620.0/			
PLOG/1.000E+02	2.29E+24	-3.25	34590.0/	! fit btw. 500 and 1800 K with MAE of 0.6%, 1.0%		
C₈H₁₇ (2-octyl) → C₇H₁₄ (1-heptene) + CH₃				5.80E+41	-8.31	52280.0
PLOG/3.000E-02	1.84E+76	-19.83	53450.0/	! fit btw. 500 and 800 K with MAE of 3.2%, 5.1%		
PLOG/3.947E-02	3.88E+70	-18.00	51780.0/	! fit btw. 500 and 800 K with MAE of 2.5%, 4.0%		
PLOG/1.000E+00	4.68E+64	-15.53	55340.0/	! fit btw. 500 and 1100 K with MAE of 7.8%, 16.0%		
PLOG/1.000E+01	1.54E+54	-12.09	54870.0/	! fit btw. 500 and 1400 K with MAE of 17.9%, 34.1%		
PLOG/1.000E+02	5.80E+41	-8.31	52280.0/	! fit btw. 500 and 1800 K with MAE of 26.1%, 57.6%		
PLOG/3.000E-02	1.84E+76	-19.83	53450.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 3.2%, 5.1%		
PLOG/3.947E-02	3.88E+70	-18.00	51780.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 2.5%, 4.0%		
PLOG/1.000E+00	1.03E+93	-23.89	70370.0/			
PLOG/1.000E+00	3.59E+62	-15.50	50750.0/	! fit btw. 500 and 1100 K with MAE of 0.5%, 1.2%		
PLOG/1.000E+01	3.38E+106	-27.33	85320.0/			
PLOG/1.000E+01	3.00E+40	-8.27	46890.0/	! fit btw. 500 and 1400 K with MAE of 0.7%, 1.4%		
PLOG/1.000E+02	8.97E+82	-20.02	80160.0/			
PLOG/1.000E+02	6.70E+31	-5.74	45010.0/	! fit btw. 500 and 1800 K with MAE of 2.2%, 4.4%		

C₈H₁₇ (2-octyl) → C₄H₈ (1-butene) + C₄H₉				3.37E+41	-8.27	51360.0
PLOG/3.000E-02	1.25E+75	-19.45	52330.0/	! fit btw. 500 and 800 K with MAE of 3.1%, 4.9%		
PLOG/3.947E-02	5.08E+69	-17.72	50770.0/	! fit btw. 500 and 800 K with MAE of 2.4%, 3.8%		
PLOG/1.000E+00	1.38E+64	-15.37	54430.0/	! fit btw. 500 and 1100 K with MAE of 7.7%, 15.9%		
PLOG/1.000E+01	5.50E+53	-11.98	53920.0/	! fit btw. 500 and 1400 K with MAE of 17.7%, 33.6%		
PLOG/1.000E+02	3.37E+41	-8.27	51360.0/	! fit btw. 500 and 1800 K with MAE of 25.7%, 56.5%		
PLOG/3.000E-02	1.25E+75	-19.45	52330.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 3.1%, 4.9%		
PLOG/3.947E-02	5.08E+69	-17.72	50770.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 2.4%, 3.8%		
PLOG/1.000E+00	6.56E+84	-21.48	65090.0/			
PLOG/1.000E+00	1.95E+58	-14.57	46270.0/	! fit btw. 500 and 1100 K with MAE of 0.9%, 2.0%		
PLOG/1.000E+01	7.16E+105	-27.15	84250.0/			
PLOG/1.000E+01	1.78E+40	-8.21	46050.0/	! fit btw. 500 and 1400 K with MAE of 0.7%, 1.5%		
PLOG/1.000E+02	6.49E+85	-20.87	81200.0/			
PLOG/1.000E+02	6.02E+30	-5.41	43970.0/	! fit btw. 500 and 1800 K with MAE of 2.1%, 4.7%		
C₈H₁₇ (2-octyl) → C₆H₁₂ (1-hexene) + C₂H₅				2.55E+41	-8.11	54520.0
PLOG/3.000E-02	2.90E+105	-28.57	66970.0/	! fit btw. 500 and 800 K with MAE of 4.7%, 7.4%		
PLOG/3.947E-02	5.40E+95	-25.47	64020.0/	! fit btw. 500 and 800 K with MAE of 3.8%, 6.1%		
PLOG/1.000E+00	2.84E+68	-16.56	59390.0/	! fit btw. 500 and 1100 K with MAE of 12.2%, 25.6%		
PLOG/1.000E+01	7.00E+54	-12.22	57390.0/	! fit btw. 500 and 1400 K with MAE of 20.7%, 41.0%		
PLOG/1.000E+02	2.55E+41	-8.11	54520.0/	! fit btw. 500 and 1800 K with MAE of 28.8%, 67.4%		
PLOG/3.000E-02	2.90E+105	-28.57	66970.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 4.7%, 7.4%		
PLOG/3.947E-02	5.40E+95	-25.47	64020.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 3.8%, 6.1%		
PLOG/1.000E+00	2.81E+150	-40.95	101000.0/			
PLOG/1.000E+00	3.31E+52	-11.94	51370.0/	! fit btw. 500 and 1100 K with MAE of 0.2%, 0.4%		
PLOG/1.000E+01	8.57E+113	-29.44	91440.0/			
PLOG/1.000E+01	8.92E+37	-7.46	47900.0/	! fit btw. 500 and 1400 K with MAE of 0.8%, 1.8%		
PLOG/1.000E+02	5.07E+88	-21.59	86020.0/			
PLOG/1.000E+02	2.39E+27	-4.31	45420.0/	! fit btw. 500 and 1800 K with MAE of 2.2%, 5.2%		

C₈H₁₇ (2-octyl) → C₅H₁₀ (1-pentene) + C₃H₇				2.92E+41	-8.15	54840.0
PLOG/3.000E-02	4.79E+105	-28.67	67270.0/	! fit btw. 500 and 800 K with MAE of 4.6%, 7.4%		
PLOG/3.947E-02	9.46E+95	-25.58	64340.0/	! fit btw. 500 and 800 K with MAE of 3.8%, 6.1%		
PLOG/1.000E+00	4.59E+68	-16.65	59740.0/	! fit btw. 500 and 1100 K with MAE of 12.2%, 25.6%		
PLOG/1.000E+01	9.44E+54	-12.28	57720.0/	! fit btw. 500 and 1400 K with MAE of 20.7%, 41.0%		
PLOG/1.000E+02	2.92E+41	-8.15	54840.0/	! fit btw. 500 and 1800 K with MAE of 28.9%, 67.6%		
PLOG/3.000E-02	4.79E+105	-28.67	67270.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 4.6%, 7.4%		
PLOG/3.947E-02	9.46E+95	-25.58	64340.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 800 K with MAE of 3.8%, 6.1%		
PLOG/1.000E+00	1.05E+106	-27.69	79120.0/			
PLOG/1.000E+00	3.98E+65	-16.50	53670.0/	! fit btw. 500 and 1100 K with MAE of 1.2%, 2.0%		
PLOG/1.000E+01	1.29E+114	-29.52	91790.0/			
PLOG/1.000E+01	1.09E+38	-7.50	48210.0/	! fit btw. 500 and 1400 K with MAE of 0.9%, 2.1%		
PLOG/1.000E+02	5.75E+88	-21.62	86340.0/			
PLOG/1.000E+02	2.51E+27	-4.34	45710.0/	! fit btw. 500 and 1800 K with MAE of 2.2%, 5.2%		
C₈H₁₇ (3-octyl) → C₂H₄ + C₆H₁₃				8.48E+40	-8.25	53720.0
PLOG/3.000E-02	3.66E+80	-21.12	58460.0/	! fit btw. 500 and 1100 K with MAE of 9.0%, 17.1%		
PLOG/3.947E-02	2.25E+78	-20.39	57980.0/	! fit btw. 500 and 1100 K with MAE of 8.7%, 17.2%		
PLOG/1.000E+00	3.57E+63	-15.39	56710.0/	! fit btw. 500 and 1300 K with MAE of 9.2%, 20.3%		
PLOG/1.000E+01	9.89E+50	-11.34	55190.0/	! fit btw. 500 and 1500 K with MAE of 16.8%, 30.4%		
PLOG/1.000E+02	8.48E+40	-8.25	53720.0/	! fit btw. 500 and 1800 K with MAE of 26.0%, 56.1%		
PLOG/3.000E-02	2.73E+88	-23.54	61590.0/			
PLOG/3.000E-02	4.68E+88	-12.13	239200.0/	! fit btw. 500 and 1100 K with MAE of 5.1%, 13.0%		
PLOG/3.947E-02	6.86E+85	-22.69	60960.0/			
PLOG/3.947E-02	8.62E+86	-11.17	244900.0/	! fit btw. 500 and 1100 K with MAE of 4.6%, 11.1%		
PLOG/1.000E+00	5.59E+71	-17.80	61100.0/			
PLOG/1.000E+00	3.15E+29	-23.32	-69440.0/	! fit btw. 500 and 1300 K with MAE of 4.4%, 14.9%		
PLOG/1.000E+01	7.65E+10	-14.11	-53320.0/			
PLOG/1.000E+01	1.94E+57	-13.15	58930.0/	! fit btw. 500 and 1500 K with MAE of 10.0%, 28.7%		
PLOG/1.000E+02	2.43E+83	-20.31	82560.0/			
PLOG/1.000E+02	6.04E+31	-5.90	46890.0/	! fit btw. 500 and 1800 K with MAE of 2.2%, 4.8%		

C₈H₁₇ (3-octyl) → C₃H₆ + C₅H₁₁				2.74E+40	-7.89	50550.0
PLOG/3.000E-02	3.42E+73	-18.87	51780.0/	! fit btw. 500 and 1100 K with MAE of 4.0%, 8.7%		
PLOG/3.947E-02	1.32E+73	-18.69	51970.0/	! fit btw. 500 and 1100 K with MAE of 3.8%, 7.9%		
PLOG/1.000E+00	1.04E+60	-14.06	52420.0/	! fit btw. 500 and 1300 K with MAE of 6.7%, 16.4%		
PLOG/1.000E+01	4.91E+46	-9.80	50520.0/	! fit btw. 500 and 1500 K with MAE of 20.7%, 51.3%		
PLOG/1.000E+02	2.74E+40	-7.89	50550.0/	! fit btw. 500 and 1800 K with MAE of 25.0%, 54.8%		
PLOG/3.000E-02	4.08E+80	-20.97	55280.0/			
PLOG/3.000E-02	1.30E+65	-18.78	34260.0/	! fit btw. 500 and 1100 K with MAE of 2.1%, 5.6%		
PLOG/3.947E-02	8.69E+81	-21.30	56440.0/			
PLOG/3.947E-02	2.08E+66	-18.08	41120.0/	! fit btw. 500 and 1100 K with MAE of 1.4%, 3.6%		
PLOG/1.000E+00	1.61E+64	-15.29	54650.0/			
PLOG/1.000E+00	4.77E+44	-17.59	-3139.0/	! fit btw. 500 and 1300 K with MAE of 5.4%, 18.3%		
PLOG/1.000E+01	1.91E+54	-12.00	54870.0/			
PLOG/1.000E+01	2.66E+36	-10.39	23890.0/	! fit btw. 500 and 1500 K with MAE of 14.7%, 45.5%		
PLOG/1.000E+02	6.59E+83	-20.23	79780.0/			
PLOG/1.000E+02	6.51E+29	-5.07	43260.0/	! fit btw. 500 and 1800 K with MAE of 2.0%, 4.4%		
C₈H₁₇ (3-octyl) → C₇H₁₄ (1-heptene) + CH₃				1.42E+27	-4.02	37990.0
PLOG/3.000E-02	5.32E+70	-18.12	51020.0/	! fit btw. 500 and 1100 K with MAE of 5.1%, 11.0%		
PLOG/3.947E-02	1.37E+69	-17.60	50570.0/	! fit btw. 500 and 1100 K with MAE of 5.3%, 11.7%		
PLOG/1.000E+00	1.14E+50	-11.33	45270.0/	! fit btw. 500 and 1300 K with MAE of 9.2%, 15.1%		
PLOG/1.000E+01	7.33E+38	-7.68	42170.0/	! fit btw. 500 and 1500 K with MAE of 13.2%, 34.2%		
PLOG/1.000E+02	1.42E+27	-4.02	37990.0/	! fit btw. 500 and 1800 K with MAE of 10.2%, 18.1%		
PLOG/3.000E-02	2.23E+80	-20.98	55790.0/			
PLOG/3.000E-02	2.11E+62	-17.99	33530.0/	! fit btw. 500 and 1100 K with MAE of 2.3%, 6.0%		
PLOG/3.947E-02	1.87E+81	-21.20	56690.0/			
PLOG/3.947E-02	1.75E+62	-17.06	38850.0/	! fit btw. 500 and 1100 K with MAE of 1.8%, 4.4%		
PLOG/1.000E+00	1.14E+121	-32.24	84630.0/			
PLOG/1.000E+00	3.31E+42	-9.16	41260.0/	! fit btw. 500 and 1300 K with MAE of 1.9%, 6.1%		
PLOG/1.000E+01	2.36E+74	-17.84	65580.0/			
PLOG/1.000E+01	1.04E+46	-10.19	42900.0/	! fit btw. 500 and 1500 K with MAE of 3.6%, 11.0%		
PLOG/1.000E+02	4.67E+59	-13.29	61010.0/			
PLOG/1.000E+02	1.84E+24	-3.31	35590.0/	! fit btw. 500 and 1800 K with MAE of 0.7%, 1.3%		

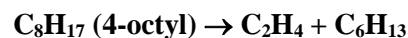
C₈H₁₇ (3-octyl) → C₄H₈ (1-butene) + C₄H₉				6.78E+26	-3.95	36920.0
PLOG/3.000E-02	1.95E+69	-17.67	49710.0/	! fit btw. 500 and 1100 K with MAE of 5.2%, 11.3%		
PLOG/3.947E-02	5.13E+67	-17.16	49250.0/	! fit btw. 500 and 1100 K with MAE of 5.5%, 11.9%		
PLOG/1.000E+00	1.77E+49	-11.09	44100.0/	! fit btw. 500 and 1300 K with MAE of 9.0%, 14.6%		
PLOG/1.000E+01	1.90E+38	-7.52	41030.0/	! fit btw. 500 and 1500 K with MAE of 13.0%, 34.0%		
PLOG/1.000E+02	6.78E+26	-3.95	36920.0/	! fit btw. 500 and 1800 K with MAE of 9.7%, 17.2%		
PLOG/3.000E-02	6.18E+79	-20.79	54940.0/			
PLOG/3.000E-02	5.35E+61	-17.40	34950.0/	! fit btw. 500 and 1100 K with MAE of 2.3%, 5.9%		
PLOG/3.947E-02	1.22E+81	-21.12	56040.0/			
PLOG/3.947E-02	1.58E+61	-16.50	39030.0/	! fit btw. 500 and 1100 K with MAE of 1.8%, 4.8%		
PLOG/1.000E+00	6.95E+70	-17.36	56910.0/			
PLOG/1.000E+00	1.35E+49	-11.54	41020.0/	! fit btw. 500 and 1300 K with MAE of 2.3%, 8.6%		
PLOG/1.000E+01	1.14E+74	-17.75	64710.0/			
PLOG/1.000E+01	3.61E+45	-10.06	41890.0/	! fit btw. 500 and 1500 K with MAE of 3.7%, 11.0%		
PLOG/1.000E+02	1.64E+59	-13.18	59910.0/			
PLOG/1.000E+02	1.33E+24	-3.29	34660.0/	! fit btw. 500 and 1800 K with MAE of 0.6%, 1.2%		
C₈H₁₇ (3-octyl) → C₆H₁₂ (1-hexene) + C₂H₅				5.07E+59	-13.58	68890.0
PLOG/1.000E-02	6.25E+80	-21.18	55340.0/	! fit btw. 500 and 1000 K with MAE of 6.3%, 11.9%		
PLOG/3.000E-02	1.68E+85	-22.26	59590.0/	! fit btw. 500 and 1100 K with MAE of 11.5%, 25.1%		
PLOG/1.000E+00	5.99E+85	-21.71	68820.0/	! fit btw. 500 and 1300 K with MAE of 12.7%, 32.7%		
PLOG/1.000E+01	1.26E+73	-17.61	69690.0/	! fit btw. 500 and 1500 K with MAE of 29.0%, 59.1%		
PLOG/1.000E+02	5.07E+59	-13.58	68890.0/	! fit btw. 500 and 1800 K with MAE of 45.9%, 122.3%		
PLOG/3.000E-02	3.28E+97	-26.03	64480.0/			
PLOG/3.000E-02	7.90E+91	-13.93	222200.0/	! fit btw. 500 and 1100 K with MAE of 4.5%, 12.3%		
PLOG/3.947E-02	4.77E+96	-25.71	64750.0/			
PLOG/3.947E-02	2.49E+91	-13.27	229300.0/	! fit btw. 500 and 1100 K with MAE of 3.9%, 9.5%		
PLOG/1.000E+00	1.39E+94	-24.17	73290.0/			
PLOG/1.000E+00	3.76E+70	-25.22	13060.0/	! fit btw. 500 and 1300 K with MAE of 9.6%, 36.9%		
PLOG/1.000E+01	-1.65E+78	-19.50	66420.0/			
PLOG/1.000E+01	1.39E+67	-16.01	62600.0/	! fit btw. 500 and 1500 K with MAE of 20.0%, 67.2%		
PLOG/1.000E+02	1.89E+38	-7.73	55240.0/			
PLOG/1.000E+02	8.28E+119	-30.71	108700.0/	! fit btw. 500 and 1800 K with MAE of 4.1%, 11.1%		



4.84E+59 -13.59 69150.0

PLOG/3.000E-02	2.79E+85	-22.36	59900.0/	! fit btw. 500 and 1100 K with MAE of 11.4%, 24.7%
PLOG/3.947E-02	2.53E+84	-21.98	60090.0/	! fit btw. 500 and 1100 K with MAE of 11.2%, 25.7%
PLOG/1.000E+00	6.84E+85	-21.76	69070.0/	! fit btw. 500 and 1300 K with MAE of 12.6%, 32.5%
PLOG/1.000E+01	1.33E+73	-17.64	69950.0/	! fit btw. 500 and 1500 K with MAE of 29.0%, 59.1%
PLOG/1.000E+02	4.84E+59	-13.59	69150.0/	! fit btw. 500 and 1800 K with MAE of 45.9%, 122.4%

PLOG/3.000E-02	3.90E+97	-26.09	64730.0/	
PLOG/3.000E-02	1.10E+92	-14.05	221800.0/	! fit btw. 500 and 1100 K with MAE of 4.6%, 12.0%
PLOG/3.947E-02	5.72E+96	-25.77	65000.0/	
PLOG/3.947E-02	3.88E+91	-13.39	229100.0/	! fit btw. 500 and 1100 K with MAE of 3.8%, 9.4%
PLOG/1.000E+00	1.57E+94	-24.21	73540.0/	
PLOG/1.000E+00	4.35E+70	-25.27	13340.0/	! fit btw. 500 and 1300 K with MAE of 9.5%, 36.1%
PLOG/1.000E+01	-1.74E+78	-19.53	66680.0/	
PLOG/1.000E+01	1.47E+67	-16.04	62870.0/	! fit btw. 500 and 1500 K with MAE of 20.0%, 66.3%
PLOG/1.000E+02	1.68E+38	-7.73	55480.0/	
PLOG/1.000E+02	8.25E+119	-30.73	109000.0/	! fit btw. 500 and 1800 K with MAE of 4.2%, 11.0%



2.72E+45 -9.46 54630.0

PLOG/3.000E-02	1.56E+68	-17.48	50970.0/	! fit btw. 500 and 1000 K with MAE of 2.4%, 6.0%
PLOG/3.947E-02	4.81E+68	-17.57	51550.0/	! fit btw. 500 and 1000 K with MAE of 2.4%, 5.7%
PLOG/1.000E+00	9.73E+59	-14.25	53600.0/	! fit btw. 500 and 1300 K with MAE of 11.4%, 40.1%
PLOG/1.000E+01	2.83E+48	-10.45	52840.0/	! fit btw. 500 and 1500 K with MAE of 23.9%, 67.8%
PLOG/1.000E+02	2.72E+45	-9.46	54630.0/	! fit btw. 500 and 1800 K with MAE of 26.2%, 58.0%

PLOG/3.000E-02	1.56E+68	-17.48	50970.0/	
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 2.4%, 6.0%
PLOG/3.947E-02	4.81E+68	-17.57	51550.0/	
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 2.4%, 5.7%
PLOG/1.000E+00	1.82E+59	-12.45	85370.0/	
PLOG/1.000E+00	3.89E+63	-15.35	55010.0/	! fit btw. 500 and 1300 K with MAE of 9.4%, 29.8%
PLOG/1.000E+01	4.97E+53	-11.97	55850.0/	
PLOG/1.000E+01	6.50E+32	-13.88	-3316.0/	! fit btw. 500 and 1500 K with MAE of 19.6%, 64.1%
PLOG/1.000E+02	1.15E+88	-21.58	83450.0/	
PLOG/1.000E+02	1.70E+35	-6.80	47300.0/	! fit btw. 500 and 1800 K with MAE of 2.0%, 4.5%

C₈H₁₇ (4-octyl) → C₃H₆ + C₅H₁₁				1.42E+42	-8.32	54840.0
PLOG/3.000E-02	1.54E+88	-23.17	60590.0/	! fit btw. 500 and 1000 K with MAE of 3.6%, 9.0%		
PLOG/3.947E-02	1.40E+89	-23.40	61570.0/	! fit btw. 500 and 1000 K with MAE of 3.8%, 8.7%		
PLOG/1.000E+00	1.43E+72	-17.73	60470.0/	! fit btw. 500 and 1300 K with MAE of 24.7%, 108.9%		
PLOG/1.000E+01	3.81E+54	-12.13	57210.0/	! fit btw. 500 and 1500 K with MAE of 21.3%, 40.8%		
PLOG/1.000E+02	1.42E+42	-8.32	54840.0/	! fit btw. 500 and 1800 K with MAE of 29.4%, 69.1%		
PLOG/3.000E-02	1.54E+88	-23.17	60590.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 3.6%, 9.0%		
PLOG/3.947E-02	1.40E+89	-23.40	61570.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 3.8%, 8.7%		
PLOG/1.000E+00	1.31E+71	-15.36	100300.0/			
PLOG/1.000E+00	4.84E+75	-18.82	61800.0/	! fit btw. 500 and 1300 K with MAE of 23.3%, 88.2%		
PLOG/1.000E+01	1.90E+54	-12.13	57210.0/			
PLOG/1.000E+01	1.90E+54	-12.13	57210.0/	! fit btw. 500 and 1500 K with MAE of 21.3%, 40.8%		
PLOG/1.000E+02	1.07E+90	-21.96	86730.0/			
PLOG/1.000E+02	8.52E+27	-4.46	45620.0/	! fit btw. 500 and 1800 K with MAE of 2.3%, 5.4%		
C₈H₁₇ (4-octyl) → C₇H₁₄ (1-heptene) + CH₃				3.34E+58	-13.22	69530.0
PLOG/3.000E-02	1.87E+90	-23.88	62340.0/	! fit btw. 500 and 1000 K with MAE of 3.6%, 9.0%		
PLOG/3.947E-02	7.47E+91	-24.30	63650.0/	! fit btw. 500 and 1000 K with MAE of 3.7%, 8.7%		
PLOG/1.000E+00	1.47E+89	-22.90	70250.0/	! fit btw. 500 and 1300 K with MAE of 100.8%, 695.5%		
PLOG/1.000E+01	4.00E+78	-19.29	73100.0/	! fit btw. 500 and 1400 K with MAE of 32.0%, 66.8%		
PLOG/1.000E+02	3.34E+58	-13.22	69530.0/	! fit btw. 500 and 1800 K with MAE of 47.6%, 127.0%		
PLOG/3.000E-02	1.87E+90	-23.88	62340.0/			
PLOG/3.000E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 3.6%, 9.0%		
PLOG/3.947E-02	7.47E+91	-24.30	63650.0/			
PLOG/3.947E-02	0.00E+00	0.00	0.0/	! fit btw. 500 and 1000 K with MAE of 3.7%, 8.7%		
PLOG/1.000E+00	1.88E+88	-20.10	116000.0/			
PLOG/1.000E+00	3.60E+92	-24.02	70980.0/	! fit btw. 500 and 1300 K with MAE of 82.9%, 499.1%		
PLOG/1.000E+01	-2.44E+103	-25.14	108000.0/			
PLOG/1.000E+01	2.31E+41	-7.90	58030.0/	! fit btw. 500 and 1400 K with MAE of 13.6%, 32.0%		
PLOG/1.000E+02	2.65E+37	-7.48	55920.0/			
PLOG/1.000E+02	2.15E+120	-30.80	110500.0/	! fit btw. 500 and 1800 K with MAE of 4.4%, 11.9%		

C₈H₁₇ (4-octyl) → C₄H₈ (1-butene) + C₄H₉				3.36E+58	-13.24	68840.0
PLOG/3.000E-02	9.80E+89	-23.77	61720.0/	! fit btw. 500 and 1000 K with MAE of 3.6%, 9.1%		
PLOG/3.947E-02	3.82E+91	-24.19	63030.0/	! fit btw. 500 and 1000 K with MAE of 3.7%, 8.8%		
PLOG/1.000E+00	1.45E+89	-22.91	69640.0/	! fit btw. 500 and 1300 K with MAE of 110.0%, 771.3%		
PLOG/1.000E+01	3.26E+78	-19.27	72440.0/	! fit btw. 500 and 1400 K with MAE of 32.0%, 66.8%		
PLOG/1.000E+02	3.36E+58	-13.24	68840.0/	! fit btw. 500 and 1800 K with MAE of 47.4%, 126.2%		
PLOG/3.000E-02	6.18E+79	-20.79	54940.0/			
PLOG/3.000E-02	5.35E+61	-17.40	34950.0/	! fit btw. 500 and 1100 K with MAE of 2.3%, 5.9%		
PLOG/3.947E-02	1.22E+81	-21.12	56040.0/			
PLOG/3.947E-02	1.58E+61	-16.50	39030.0/	! fit btw. 500 and 1100 K with MAE of 1.8%, 4.8%		
PLOG/1.000E+00	6.95E+70	-17.36	56910.0/			
PLOG/1.000E+00	1.35E+49	-11.54	41020.0/	! fit btw. 500 and 1300 K with MAE of 2.3%, 8.6%		
PLOG/1.000E+01	1.14E+74	-17.75	64710.0/			
PLOG/1.000E+01	3.61E+45	-10.06	41890.0/	! fit btw. 500 and 1500 K with MAE of 3.7%, 11.0%		
PLOG/1.000E+02	1.64E+59	-13.18	59910.0/			
PLOG/1.000E+02	1.33E+24	-3.29	34660.0/	! fit btw. 500 and 1800 K with MAE of 0.6%, 1.2%		
C₈H₁₇ (4-octyl) → C₆H₁₂ (1-hexene) + C₂H₅				5.07E+59	-13.58	68890.0
PLOG/3.000E-02	1.68E+85	-22.26	59590.0/	! fit btw. 500 and 1100 K with MAE of 11.5%, 25.1%		
PLOG/3.947E-02	1.49E+84	-21.88	59780.0/	! fit btw. 500 and 1100 K with MAE of 11.4%, 26.0%		
PLOG/1.000E+00	5.99E+85	-21.71	68820.0/	! fit btw. 500 and 1300 K with MAE of 12.7%, 32.7%		
PLOG/1.000E+01	1.26E+73	-17.61	69690.0/	! fit btw. 500 and 1500 K with MAE of 29.0%, 59.1%		
PLOG/1.000E+02	5.07E+59	-13.58	68890.0/	! fit btw. 500 and 1800 K with MAE of 45.9%, 122.3%		
PLOG/3.000E-02	3.28E+97	-26.03	64480.0/			
PLOG/3.000E-02	7.90E+91	-13.93	222200.0/	! fit btw. 500 and 1100 K with MAE of 4.5%, 12.3%		
PLOG/3.947E-02	4.77E+96	-25.71	64750.0/			
PLOG/3.947E-02	2.49E+91	-13.27	229300.0/	! fit btw. 500 and 1100 K with MAE of 3.9%, 9.5%		
PLOG/1.000E+00	1.39E+94	-24.17	73290.0/			
PLOG/1.000E+00	3.76E+70	-25.22	13060.0/	! fit btw. 500 and 1300 K with MAE of 9.6%, 36.9%		
PLOG/1.000E+01	-1.65E+78	-19.50	66420.0/			
PLOG/1.000E+01	1.39E+67	-16.01	62600.0/	! fit btw. 500 and 1500 K with MAE of 20.0%, 67.2%		
PLOG/1.000E+02	1.89E+38	-7.73	55240.0/			
PLOG/1.000E+02	8.28E+119	-30.71	108700.0/	! fit btw. 500 and 1800 K with MAE of 4.1%, 11.1%		

C₈H₁₇ (4-octyl) → C₅H₁₀ (1-pentene) + C₃H₇				4.84E+59	-13.59	69150.0
PLOG/3.000E-02	2.79E+85	-22.36	59900.0/	! fit btw. 500 and 1100 K with MAE of 11.4%, 24.7%		
PLOG/3.947E-02	2.53E+84	-21.98	60090.0/	! fit btw. 500 and 1100 K with MAE of 11.2%, 25.7%		
PLOG/1.000E+00	6.84E+85	-21.76	69070.0/	! fit btw. 500 and 1300 K with MAE of 12.6%, 32.5%		
PLOG/1.000E+01	1.33E+73	-17.64	69950.0/	! fit btw. 500 and 1500 K with MAE of 29.0%, 59.1%		
PLOG/1.000E+02	4.84E+59	-13.59	69150.0/	! fit btw. 500 and 1800 K with MAE of 45.9%, 122.4%		
PLOG/3.000E-02	3.90E+97	-26.09	64730.0/			
PLOG/3.000E-02	1.10E+92	-14.05	221800.0/	! fit btw. 500 and 1100 K with MAE of 4.6%, 12.0%		
PLOG/3.947E-02	5.72E+96	-25.77	65000.0/			
PLOG/3.947E-02	3.88E+91	-13.39	229100.0/	! fit btw. 500 and 1100 K with MAE of 3.8%, 9.4%		
PLOG/1.000E+00	1.57E+94	-24.21	73540.0/			
PLOG/1.000E+00	4.35E+70	-25.27	13340.0/	! fit btw. 500 and 1300 K with MAE of 9.5%, 36.1%		
PLOG/1.000E+01	-1.74E+78	-19.53	66680.0/			
PLOG/1.000E+01	1.47E+67	-16.04	62870.0/	! fit btw. 500 and 1500 K with MAE of 20.0%, 66.3%		
PLOG/1.000E+02	1.68E+38	-7.73	55480.0/			
PLOG/1.000E+02	8.25E+119	-30.73	109000.0/	! fit btw. 500 and 1800 K with MAE of 4.2%, 11.0%		
C₁₀H₂₁ (2-decyl) → C₃H₆ + C₇H₁₅^b				2.90E+32	-5.40	40430.0
PLOG/3.000E-02	6.73E+37	-7.93	36250.0/	! fit btw. 500 and 2500 K with MAE of 36.2%, 82.4%		
PLOG/1.000E+00	1.16E+41	-8.38	41280.0/	! fit btw. 500 and 2500 K with MAE of 22.1%, 37.9%		
PLOG/1.000E+01	3.71E+38	-7.39	41980.0/	! fit btw. 500 and 2500 K with MAE of 13.8%, 21.5%		
PLOG/1.000E+02	2.90E+32	-5.40	40430.0/	! fit btw. 500 and 2500 K with MAE of 12.8%, 28.6%		
PLOG/3.000E-02	2.87E+84	-21.91	57660.0/			
PLOG/3.000E-02	2.25E+24	-4.02	31090.0/	! fit btw. 500 and 2500 K with MAE of 3.9%, 6.4%		
PLOG/1.000E+00	3.56E+53	-12.09	47270.0/			
PLOG/1.000E+00	7.45E+65	-14.42	89020.0/	! fit btw. 500 and 2500 K with MAE of 6.9%, 21.9%		
PLOG/1.000E+01	7.17E+87	-21.73	71070.0/			
PLOG/1.000E+01	1.06E+28	-4.41	36100.0/	! fit btw. 500 and 2500 K with MAE of 1.7%, 3.7%		
PLOG/1.000E+02	5.78E+77	-18.33	71580.0/			
PLOG/1.000E+02	9.82E+24	-3.33	35880.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 2.4%		
C₁₀H₂₁ (3-decyl) → C₄H₈ (1-butene) + C₆H₁₃^b				1.68E+27	-3.99	37630.0
PLOG/3.000E-02	7.60E+37	-7.95	36880.0/	! fit btw. 500 and 2500 K with MAE of 32.1%, 62.9%		

PLOG/1.000E+00	5.51E+38	-7.74	40550.0/	! fit btw. 500 and 2500 K with MAE of 16.5%, 30.9%
PLOG/1.000E+01	2.86E+34	-6.26	40100.0/	! fit btw. 500 and 2500 K with MAE of 11.1%, 21.5%
PLOG/1.000E+02	1.68E+27	-3.99	37630.0/	! fit btw. 500 and 2500 K with MAE of 11.6%, 21.3%
PLOG/3.000E-02	3.52E+83	-21.60	58370.0/	
PLOG/3.000E-02	3.21E+23	-3.81	30580.0/	! fit btw. 500 and 2500 K with MAE of 3.0%, 5.3%
PLOG/1.000E+00	1.69E+46	-9.96	44190.0/	
PLOG/1.000E+00	5.82E+90	-20.87	125300.0/	! fit btw. 500 and 2500 K with MAE of 7.0%, 19.7%
PLOG/1.000E+01	5.25E+86	-21.36	73080.0/	
PLOG/1.000E+01	1.06E+27	-4.17	35810.0/	! fit btw. 500 and 2500 K with MAE of 1.1%, 2.7%
PLOG/1.000E+02	1.08E+65	-14.70	65610.0/	
PLOG/1.000E+02	2.43E+22	-2.67	34460.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 2.4%

C₁₀H₂₁ (3-decyl) → C₉H₁₈ (1-nonene) + CH₃^b

1.69E+27 -3.99 37530.0

PLOG/3.000E-02	3.96E+37	-7.87	36600.0/	! fit btw. 500 and 2500 K with MAE of 32.0%, 63.2%
PLOG/1.000E+00	4.03E+38	-7.70	40350.0/	! fit btw. 500 and 2500 K with MAE of 16.6%, 31.0%
PLOG/1.000E+01	2.59E+34	-6.25	39960.0/	! fit btw. 500 and 2500 K with MAE of 11.2%, 21.9%
PLOG/1.000E+02	1.69E+27	-3.99	37530.0/	! fit btw. 500 and 2500 K with MAE of 11.8%, 22.0%

PLOG/3.000E-02	1.68E+83	-21.52	58050.0/	
PLOG/3.000E-02	2.08E+23	-3.75	30360.0/	! fit btw. 500 and 2500 K with MAE of 3.0%, 5.3%
PLOG/1.000E+00	1.54E+46	-9.95	44040.0/	
PLOG/1.000E+00	4.81E+89	-20.59	123800.0/	! fit btw. 500 and 2500 K with MAE of 7.0%, 20.1%
PLOG/1.000E+01	1.72E+86	-21.22	72600.0/	
PLOG/1.000E+01	6.29E+26	-4.11	35560.0/	! fit btw. 500 and 2500 K with MAE of 1.0%, 2.6%
PLOG/1.000E+02	7.63E+64	-14.66	65310.0/	
PLOG/1.000E+02	1.50E+22	-2.62	34230.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 2.4%

C₁₀H₂₁ (4-decyl) → C₅H₁₀ (1-pentene) + C₅H₁₁^b

1.03E+26 -3.66 37020.0

PLOG/3.000E-02	6.54E+37	-7.93	37010.0/	! fit btw. 500 and 2500 K with MAE of 31.0%, 57.8%
PLOG/1.000E+00	1.22E+38	-7.56	40350.0/	! fit btw. 500 and 2500 K with MAE of 15.2%, 28.9%
PLOG/1.000E+01	2.62E+33	-5.98	39640.0/	! fit btw. 500 and 2500 K with MAE of 10.7%, 22.0%
PLOG/1.000E+02	1.03E+26	-3.66	37020.0/	! fit btw. 500 and 2500 K with MAE of 11.6%, 20.2%

PLOG/3.000E-02	1.18E+83	-21.45	58470.0/	
PLOG/3.000E-02	1.98E+23	-3.75	30500.0/	! fit btw. 500 and 2500 K with MAE of 2.8%, 5.0%
PLOG/1.000E+00	3.32E+44	-9.46	43490.0/	

PLOG/1.000E+00	1.50E+101	-23.57	140100.0/	! fit btw. 500 and 2500 K with MAE of 7.2%, 19.2%
PLOG/1.000E+01	4.61E+84	-20.75	72570.0/	
PLOG/1.000E+01	2.19E+26	-3.99	35510.0/	! fit btw. 500 and 2500 K with MAE of 1.0%, 2.1%
PLOG/1.000E+02	6.34E+61	-13.78	64010.0/	
PLOG/1.000E+02	4.30E+21	-2.48	34080.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 2.3%



3.67E+28 -4.36 37720.0

PLOG/3.000E-02	5.60E+36	-7.63	35480.0/	! fit btw. 500 and 2500 K with MAE of 33.5%, 72.0%
PLOG/1.000E+00	6.44E+38	-7.77	39810.0/	! fit btw. 500 and 2500 K with MAE of 18.4%, 33.6%
PLOG/1.000E+01	2.08E+35	-6.51	39840.0/	! fit btw. 500 and 2500 K with MAE of 11.4%, 19.2%
PLOG/1.000E+02	3.67E+28	-4.36	37720.0/	! fit btw. 500 and 2500 K with MAE of 11.0%, 22.0%

PLOG/3.000E-02	1.13E+82	-21.21	56460.0/	
PLOG/3.000E-02	1.72E+23	-3.73	30000.0/	! fit btw. 500 and 2500 K with MAE of 3.4%, 5.6%
PLOG/1.000E+00	2.30E+48	-10.60	44420.0/	
PLOG/1.000E+00	2.11E+74	-16.60	102000.0/	! fit btw. 500 and 2500 K with MAE of 6.5%, 19.5%
PLOG/1.000E+01	1.75E+86	-21.29	70930.0/	
PLOG/1.000E+01	1.48E+27	-4.21	35210.0/	! fit btw. 500 and 2500 K with MAE of 1.4%, 3.5%
PLOG/1.000E+02	1.02E+69	-15.87	66740.0/	
PLOG/1.000E+02	1.44E+23	-2.88	34300.0/	! fit btw. 500 and 2500 K with MAE of 0.8%, 2.1%



6.22E+26 -3.88 37340.0

PLOG/3.000E-02	5.47E+37	-7.91	36790.0/	! fit btw. 500 and 2500 K with MAE of 31.7%, 61.5%
PLOG/1.000E+00	2.82E+38	-7.66	40370.0/	! fit btw. 500 and 2500 K with MAE of 16.1%, 30.3%
PLOG/1.000E+01	1.16E+34	-6.15	39850.0/	! fit btw. 500 and 2500 K with MAE of 10.9%, 21.5%
PLOG/1.000E+02	6.22E+26	-3.88	37340.0/	! fit btw. 500 and 2500 K with MAE of 11.5%, 20.8%

PLOG/3.000E-02	1.62E+83	-21.50	58220.0/	
PLOG/3.000E-02	2.39E+23	-3.77	30470.0/	! fit btw. 500 and 2500 K with MAE of 2.9%, 5.1%
PLOG/1.000E+00	4.33E+45	-9.79	43870.0/	
PLOG/1.000E+00	9.64E+92	-21.45	128500.0/	! fit btw. 500 and 2500 K with MAE of 7.0%, 19.6%
PLOG/1.000E+01	8.22E+83	-20.55	71450.0/	
PLOG/1.000E+01	3.61E+26	-4.05	35500.0/	! fit btw. 500 and 2500 K with MAE of 1.0%, 2.5%
PLOG/1.000E+02	8.81E+63	-14.40	64990.0/	
PLOG/1.000E+02	1.32E+22	-2.61	34260.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 2.2%

C₁₀H₂₁ (5-decyl) → C₇H₁₄ (1-heptene) + C₃H₇^b				1.48E+27	-3.98	37490.0
PLOG/3.000E-02	4.77E+37	-7.89	36670.0/	! fit btw. 500 and 2500 K with MAE of 32.1%, 63.4%		
PLOG/1.000E+00	4.08E+38	-7.71	40370.0/	! fit btw. 500 and 2500 K with MAE of 16.5%, 31.0%		
PLOG/1.000E+01	2.34E+34	-6.24	39940.0/	! fit btw. 500 and 2500 K with MAE of 11.0%, 21.2%		
PLOG/1.000E+02	1.48E+27	-3.98	37490.0/	! fit btw. 500 and 2500 K with MAE of 11.5%, 21.1%		
PLOG/3.000E-02	1.91E+83	-21.53	58100.0/			
PLOG/3.000E-02	2.62E+23	-3.78	30450.0/	! fit btw. 500 and 2500 K with MAE of 3.0%, 5.2%		
PLOG/1.000E+00	1.52E+46	-9.95	44050.0/			
PLOG/1.000E+00	2.60E+89	-20.52	123500.0/	! fit btw. 500 and 2500 K with MAE of 6.9%, 19.6%		
PLOG/1.000E+01	2.21E+84	-20.68	71410.0/			
PLOG/1.000E+01	5.31E+26	-4.09	35530.0/	! fit btw. 500 and 2500 K with MAE of 1.1%, 2.7%		
PLOG/1.000E+02	9.63E+64	-14.69	65450.0/			
PLOG/1.000E+02	2.25E+22	-2.67	34340.0/	! fit btw. 500 and 2500 K with MAE of 0.9%, 2.4%		

^aFits have been carried out using the auxiliary MESS_TPfit code written by Franklin Goldsmith; see <http://tcg.cse.anl.gov/papr/codes/mess.html>.

^bThe calculations of the rate constant have been performed using a simplified PES including only the direct C-C bond β -scission channel.

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