

# Enthalpies of Decalins and of *trans*-Decalin and *n*-Pentane Mixtures

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Measured enthalpy values are reported for pure Decalins and four mixtures of *trans*-Decalin and *n*-pentane.

With the use of a flow calorimeter the enthalpies of both *trans*- and *cis*-Decalin (decahydronaphthalene) have been measured from 75° to 620° F. with pressures up to 1400 p.s.i.a. In addition, enthalpy values have been determined for mixtures of *trans*-Decalin with *n*-pentane, containing 19.9, 40.0, 57.9, and 80.0 weight % pentane. Previously Seyer (9) presented thermal measurements of both pure *cis*- and pure *trans*-Decalin in the liquid state up to 275° F. Seyer and Mann (10) measured the latent heat of vaporization at atmospheric pressure. McCullough, Finke, Messerly, Todd, Kincheloe, and Waddington (7) presented enthalpy values for liquid and solid phases from very low temperatures up to 175° F. Vvendenskii and Maioron (11) show heat capacities for the pure Decalins in the ideal gas state of zero pressure. Findl, Brande, and Edwards (4) report enthalpy values and latent heats of vaporization for a commercially impure mixture containing *cis*- and *trans*-Decalins. In general, a more thorough measurement study of the enthalpy for the pure components is needed. Enthalpy measurements for the mixture of pentane with *trans*-Decalin have not previously been made.

A total of 955 measurements were made on the pure Decalins and the pentane-Decalin mixtures, and are available from the American Society for Information Science (ASIS). These deposited measurements show the enthalpy relative to 75° F. and the pressure of measurement. The calorimeter measurements were previously shown to give results with an average deviation of 1.5 B.t.u. per pound, as compared with literature values for pentane (2) and liquid water (8).

The Decalin was obtained as a mixture of *cis* and *trans* isomers. The mixture was purified by fractional distillation using a 40 to 1 reflux ratio with a laboratory column having approximately 20 theoretical stages. The portion of the distillate selected as pure *trans*-Decalin had a refractive index of  $1.46934n_D^{20}$  and a density of 0.8680 at 72° F. Corresponding values shown in the literature (2) are 1.4695 and 0.8682. For the *cis*-Decalin the measured values are  $1.48037n_D^{20}$  with a density of 0.9005 at 60° F., with literature values of 1.4810 and 0.9002. The purity of these Decalin components is considered to be better than 95%, with the majority impurity the other isomer. The *n*-pentane used has a purity determined by chromatograph to exceed 99.9%.

To place the measurements on the API data book (1) basis of -200° F. and the pure saturated liquid state, it is necessary to establish the enthalpy difference between -200° and 75° F. McCullough *et al.* (7) show enthalpy values

Table I. Properties of Liquid Phase at 75° F. and 1 Atm. for *trans*-Decalin Systems with *n*-Pentane

Material	Wt. % <i>n</i> -Pentane	Liquid Density, G./Cm. <sup>3</sup>	Heat of Mixing, B.t.u./ Lb.	Enthalpy to Add, B.t.u./Lb.
100% <i>trans</i> -Decalin	0	0.8664	0	91.1
32.2 Mole % pentane	19.9	0.8105	0.16	98.4
56.1 Mole % pentane	40.0	0.7577	0.21	106.1
72.5 Mole % pentane	57.9	0.7094	0.17	112.9
88.4 Mole % pentane	80.0	0.6639	0.08	121.5
100 % <i>cis</i> -Decalin	0	0.8928	0	90.2
100 % <i>n</i> -Pentane	100	0.6219	0	129.4

Table II. Smoothed Values of Enthalpy for *cis*-Decalin

Temp., ° F.	Units. B.t.u. per lb. Base level. Pure saturated liquid at -200° F.					
	P.S.I.A.					
	0	25	40	70	100	1400
75		90.2	90.2	90.3	90.4	93.6
120		108.4				112.1
160		125.6				129.4
200		143.9				148.0
240		163.2				167.6
280		184.7				188.2
320		206.7				209.7
360		229.3				232.3
400		253.3				256.1
420		265.8				268.5
431.2		272.8 <sup>a</sup>				
431.2		390.0 <sup>a</sup>				
440		395.0	278.3			281.1
460	409.1	406.3	291.2			293.7
479.5			304.3 <sup>a</sup>			
479.5			415.5 <sup>a</sup>			
480	420.5	417.8	415.7	306.3		304.7
500	432.4	429.8	427.7	318.6		319.1
520	444.4	442.2	439.9	332.3		332.3
532.2				341.5 <sup>a</sup>		
532.2				443.1 <sup>a</sup>		
540	457.2	454.6	452.3	448.2	346.2	346.2
560	470.1			461.4	360.0	359.8
574.8					370.1 <sup>a</sup>	
574.8					465.3 <sup>a</sup>	
580	483.6			475.3	468.7	373.5
600	497.2				481.6	387.4

<sup>a</sup> Enthalpy value on two-phase boundary.

Table III. Smoothed Values of Enthalpy for *trans*-Decalin

Temp., ° F.	Units. B.t.u. per lb.							
	Base level. Pure saturated liquid at -200° F.							
	P.S.I.A.							
	0	22	40	70	100	150	1000	1400
75		91.1	91.1	91.2	91.3	91.5	93.9	95.1
120		109.1				109.4		112.8
160		126.8				127.1		130.0
200		145.3				145.6		148.7
240		164.8				165.1		167.7
280		185.2				185.4		187.2
320		206.3				206.5		208.2
360		228.7				228.8		230.0
380		240.3				240.4		241.3
399.5		252.0 <sup>a</sup>						
399.5		372.4 <sup>a</sup>						
400		372.6	252.2			252.3		252.9
420			264.4			264.5	265.3	
440			276.8			276.9	277.8	
455			286.6 <sup>a</sup>					
455			391.6 <sup>a</sup>					
460	398.8		394.0	289.7		289.8	290.3	
480	408.3		404.0	302.4		302.5	302.9	
500	418.7		414.2	315.5		315.5	315.5	
515				325.0 <sup>a</sup>				
515				417.3 <sup>a</sup>				
520	429.3		424.5	420.1	328.4	328.4	328.4	
540	440.1		435.3	431.1	341.7	341.7	341.7	
557.6					353.8 <sup>a</sup>			
557.6					437.2 <sup>a</sup>			
560	451.2		446.5	442.2	438.7	355.3	355.0	
580	462.5		457.2	453.2	449.8	369.6	369.0	
600	473.7		468.0	464.2	460.8	384.0	383.2	
609						391.2 <sup>a</sup>		
609						461.2 <sup>a</sup>		
620	483.9			475.3	472.1	467.3	397.9	

<sup>a</sup> Enthalpy value on two-phase boundary.Table IV. Smoothed Values of Enthalpy for Mixture of 32.2 Mole % Pentane and 67.8 Mole % *trans*-Decalin

Temp., ° F.	Units. B.t.u. per lb.											
	Base Level. Pure saturated liquid components at -200° F.											
	P.S.I.A.											
	0	20	40	70	100	150	200	300	400	600	1000	1400
75		98.4	98.4	98.5	98.6	98.7	98.9	99.1	99.4	99.9	100.9	102.0
120		118.0							119.0		120.7	121.6
160		136.4							137.2		138.5	139.4
187		149.3 <sup>a</sup>										
200		161.0	155.9						156.6		157.8	158.6
220		177.8	166.4						167.0		168.1	168.8
240		194.4	177.0						177.6		178.6	179.3
244.8			179.6 <sup>a</sup>									
260			194.1	187.8					188.4		189.5	190.2
280			210.3	198.7					199.3		200.4	201.1
300				210.0					210.5		211.5	212.2
301.6				211.6 <sup>a</sup>								
320				228.2	221.4				221.8		222.7	223.3
340				243.7	233.0				233.4		234.2	234.7
344.2					235.5 <sup>a</sup>							
360		332.5	278.7	260.8	249.9	244.7			245.1		246.0	246.6
371.8		369.8 <sup>a</sup>										
380		373.6	302.7		267.4	256.6			256.9		257.8	258.3
389.1						262.2 <sup>a</sup>						
400		383.1	334.6		285.0	271.6	268.8		269.0		269.7	270.1
420		393.2	388.0	313.0	303.2	288.9	281.8		282.0		282.5	282.9
421.3			392.2 <sup>a</sup>									
436.3							292.4 <sup>a</sup>					
440		403.6	402.0	345.5	323.0	306.8	296.2	294.8	294.7		294.2	295.9
460	416.1	414.3	412.7	383.6	345.7	325.7	313.9	308.3	308.2		307.4	308.8
470	421.2	419.8	418.4	407.4	358.7	335.5	323.0	314.8	314.7		313.9	315.2
474.3				419.3 <sup>a</sup>								
480	426.6	425.4	424.0	422.5	372.8	345.4	332.1	321.7	321.5		320.8	321.7

(continued)

Table IV. (Continued)

Temp., ° F.	Units. B.t.u. per lb. Base Level. Pure saturated liquid components at -200° F.											
	P.S.I.A.											
	0	20	40	70	100	150	200	300	400	600	1000	1400
500	437.4		435.5	434.2	411.6	366.5	351.0	335.5	333.2		333.7	334.4
509								341.8 <sup>a</sup>				
509.8					438.8 <sup>a</sup>							
520	448.4			445.9	444.3	392.6	372.1	353.1	349.7	348.6	347.8	348.0
540	459.8			457.2	455.7	426.3	395.2	373.2	364.3	362.9	361.7	361.3
557.2						462.2 <sup>a</sup>						
560	471.3				467.0	463.8	421.7	393.7	380.3	377.6	376.1	374.9
580	482.6				478.3	475.2	459.3	415.0	398.2	392.7	390.7	388.2
588.8							477.6 <sup>a</sup>					
590	488.0				483.6	480.9	478.3	426.6	406.7	400.4	398.3	394.8
600	493.7				489.3	486.7	484.4	439.3	416.0	408.2	405.9	401.5

<sup>a</sup> Enthalpy value on two-phase boundary.

Table V. Smoothed Values of Enthalpy for Mixture of 56.1 Mole % Pentane and 43.9 Mole % *trans*-Decalin

Temp., ° F.	Units. B.t.u. per lb. Base level. Pure saturated liquid components at -200° F.											
	P.S.I.A.											
	0	70	100	200	300	400	500	540	600	800	1000	1400
75		106.1	106.2	106.5	106.8	107.1	107.3	107.4	107.7	108.3	108.9	110.1
120		126.7				127.8				129.1		131.0
160		146.8				147.6				148.6		150.1
200		167.5				168.2				169.0		170.2
240		189.0				189.7				190.5		191.7
246.6		192.8 <sup>a</sup>										
260		217.7	200.6			201.1				201.8		202.9
280		241.0	212.7			213.1				213.6		214.4
282.3			214.0 <sup>a</sup>									
300		261.6	241.0	224.7		224.9				225.5		226.2
320		279.8	263.2	237.0		237.2				237.6		238.2
340		297.0	282.8	249.7		249.8				250.2		250.6
358.6				262.0 <sup>a</sup>								
360		315.5	300.9	264.2	263.0	263.0				263.0		263.0
380		336.4	319.8	288.4	275.8	275.8				275.7		275.5
400		360.8	340.2	308.7	288.7	288.7				288.5		288.2
420		390.2	362.9	328.2	301.9	301.8				301.4		301.2
423.5					304.4 <sup>a</sup>							
435.7		415.0 <sup>a</sup>										
440		417.4	388.8	347.8	324.6	315.7				315.3		314.6
460	433.3	428.5	418.5	368.6	346.7	321.1				319.9		318.0
463.2						331.3 <sup>a</sup>						
467.6			430.1 <sup>a</sup>									
480	444.2	439.9	437.5	390.6	369.0	349.4	342.7			342.4		341.7
493.2							351.7 <sup>a</sup>					
500	455.5	451.7	449.7	414.8	390.0	370.3	359.0	357.2	357.2	356.8	356.5	355.3
520	467.0	463.8	461.7	442.3	410.8	391.9	380.0	375.8	373.0	371.8	370.7	369.4
532				461.5 <sup>a</sup>								
540	478.7	475.8	473.8	466.7	435.0	414.4	401.2	395.8	391.6	386.9	385.4	384.0
560	490.6	487.7	485.8	479.8	462.1	437.8	422.9	417.7	410.7	402.7	400.7	399.0
575.8					484.1 <sup>a</sup>							
580	502.4	499.6	498.0	492.8	487.0	462.6	445.2	440.4	433.0	420.2	416.7	414.2
600	514.7	511.7	510.3	506.0	500.0	488.0	469.7	464.3	456.0	438.8	433.0	430.2

<sup>a</sup> Enthalpy value on two-phase boundary.

for this temperature range. Both isomers solidify as the temperature reduces to -200° F. By extrapolation of the *trans*-Decalin data, the condition of the supercooled liquid at -200° F. was determined to be 91.1 B.t.u. per pound less than the saturated liquid at 75° F. For the *cis*-Decalin, the difference was 90.2 B.t.u. per pound. These values are believed to be within 1.5 B.t.u. per pound of the true value. The choice of the supercooled liquid at -200° F. introduces some small uncertainty of base level, but is consistent with the base level used by the API data book for the hydrocarbons. For the mixtures of *n*-pentane and *trans*-Decalin, the enthalpy needed for addition to the

measured enthalpies is a weight average of 91.1 and 129.4 for *trans*-Decalin and *n*-pentane, respectively, plus the heat of mixing at 75° F. The heats of mixing were evaluated from the results of Lundberg (6) and Brandt (3). In addition, the small change in enthalpy from the saturated pressure to the operating pressure at 75° F. was added to the measured values. This small enthalpy change was computed as previously described (5). It was also established that the zero pressure enthalpies for various isotherms plotted linearly against weight fraction pentane. Table I shows the compositions studied, with density and heat of mixing at 75° F., and the enthalpy needed to convert the saturated

Table VI. Smoothed Values of Enthalpy for Mixture of 72.5 Mole % Pentane and 27.5 Mole % *trans*-Decalin

Temp., ° F.	Units. B.t.u. per lb. Base level. Pure saturated liquid components at -200° F.											
	P.S.I.A.											
	0	40	70	100	200	300	400	500	600	800	1000	1400
75		112.9	113.0	113.1	113.3	113.6	113.9	114.2	114.5	115.0	115.6	116.7
120		135.3					136.2			137.2		138.8
160		156.4					157.2			158.2		159.6
176.4		165.3 <sup>a</sup>										
180		177.5	167.3				168.0			169.2		170.3
200		228.5	178.3				179.0			180.2		181.4
218.4			188.7 <sup>a</sup>									
220			193.1	189.7			190.4			191.3		192.7
240			240.7	201.2			201.9			203.0		204.4
251.7				208.2 <sup>a</sup>								
260				232.0	213.3		213.8			214.9		216.6
280				269.4	226.0		226.5			227.4		228.8
300		327.3			238.9		239.3			240.1		241.4
320		349.2			252.0		252.4			253.1		254.2
325.7					255.7 <sup>a</sup>							
340		370.7	345.8		287.9	265.3	265.5			266.1		267.1
359		390.1 <sup>a</sup>										
360		390.7	367.8	353.4		278.5	278.6			279.2		280.0
377.8						290.3 <sup>a</sup>						
380		401.6	392.5	373.4		296.3	291.6			292.1		292.9
390			405.3 <sup>a</sup>									
400		412.7	411.0	397.4		330.9	305.2			305.6		306.3
414.2							314.8 <sup>a</sup>					
418.5				419.3 <sup>a</sup>								
420		424.0	422.1	420.1	382.5	356.4	326.9	319.0		319.3		319.9
440		435.3	433.6	431.7	404.2		356.4	334.2		334.1		334.0
444.1								337.6 <sup>a</sup>				
460	448.8	446.7	445.2	443.4	427.4		382.2	358.8	350.3	349.8		348.3
477					447.1 <sup>a</sup>							
480	460.0	458.4	456.9	455.3	449.0	423.0	406.0	384.7	368.8	367.3		363.0
500	471.7		469.0	467.4	461.6	445.3	428.7	409.8	393.9	382.1	380.1	377.7
517						465.0 <sup>a</sup>						
520	483.6		481.2	479.7	474.1	467.0	450.8	434.5	418.2	400.6	396.8	392.8
539							472.6 <sup>a</sup>					
540	495.6		493.5	491.8	486.6	480.1	473.3	458.1	442.0	420.2	414.0	408.1
550	501.7			498.0	492.8	486.7	479.9	470.0 <sup>a</sup>	454.0	430.6	422.7	415.8
560	507.8			504.2	499.2	493.3	486.3	477.4	465.1	440.8	431.7	423.7
600	532.8			528.9	524.4	519.0	512.2	506.0	498.4	481.1	466.8	455.8

<sup>a</sup> Enthalpy value on two-phase boundary.Table VII. Smoothed Values of Enthalpy for Mixture of 88.4 Mole % Pentane and 11.6 Mole % *trans*-Decalin

Temp., ° F.	Units. B.t.u. per lb. Base level. Pure saturated liquid components at -200° F.											
	P.S.I.A.											
	0	40	70	100	200	300	400	500	600	800	1000	1400
75		121.5	121.6	121.7	121.9	122.2	122.4	122.7	122.9	123.5	124.0	125.0
120		145.2					146.2			147.2		148.8
160.4		168.4 <sup>a</sup>										
170		214.0	174.0				174.4			174.9		175.7
180		254.4	180.0				180.3			180.7		181.2
200		284.4	191.8				191.9			192.1		192.3
203.2			193.8 <sup>a</sup>									
210		294.7	223.0	198.2			198.2			198.2		198.2
220		304.3	263.7	204.2			204.2			204.2		204.2
235.1				213.6 <sup>a</sup>								
240		322.6	297.7	237.7	216.7		216.7			216.7		216.7
250		331.0	309.0	279.2	223.1		223.1			223.1		223.1
260		339.8	319.5	299.3	229.7		229.7			229.7		229.7
280		356.8	339.7	327.0	242.7		242.7			242.7		242.7
298.9					255.4 <sup>a</sup>							
300		372.3	358.7	347.6	258.7	256.2	256.2			256.2		256.2
316		384.1										
320		386.8	377.4	366.0	317.7	269.8	269.8			269.7		269.6
337.8			394.5 <sup>a</sup>									
340		397.2	395.7	384.4	350.6	284.6	284.5			384.1		283.6
348.9						291.4 <sup>a</sup>						

(continued)

Table VII. (Continued)

Units. B.t.u. per lb.  
Base level. Pure saturated liquid components at  $-200^{\circ}\text{F}$ .

Temp., $^{\circ}\text{F}$ .	P.S.I.A.											
	0	40	70	100	200	300	400	500	600	800	1000	1400
360		408.1	406.3	404.0	373.0	324.0	300.2			299.2		297.6
361.2				405.4 <sup>a</sup>								
380		419.2	417.2	415.5	393.8	364.8	316.0			314.0		311.8
381							316.7 <sup>a</sup>					
400	432.7	430.3	428.4	426.6	414.5	389.7	358.3	331.8		329.0	327.4	326.1
409								338.0 <sup>a</sup>				
412.3					427.5 <sup>a</sup>							
420	443.7	441.8	439.8	438.1	431.7	411.3	394.0	358.3	347.7	344.4	342.7	341.2
430	449.7	447.7	445.8	443.9	437.6	421.7	407.1	377.2	356.7	352.4	350.3	348.8
440	455.6	453.5	451.8	449.9	443.6	431.6	418.4	394.7	366.7	360.7	358.2	356.6
452.7						444.5 <sup>a</sup>						
460	468.0	465.6	463.9	462.0	455.8	449.0	437.7	421.7	396.7	379.3	374.2	372.2
470	474.0	471.8	470.2	468.1	462.1	455.4	446.7	433.3	412.3	389.0	382.4	380.1
478.4							454.4 <sup>a</sup>					
480	480.0	477.9	476.4	474.3	468.3	462.0	455.6	444.2	427.4	399.3	390.7	388.0
493								456.5 <sup>a</sup>				
500	492.3	490.4	489.0	487.0	481.3	475.0	468.9	461.6	448.4	421.4	408.3	404.4
520	504.5	502.9	501.3	499.7	494.2	488.3	482.5	476.0	465.9	445.0	427.6	421.2
560	529.8			525.6	522.9	515.4	509.7	504.6	498.3	483.8	466.4	454.6
600	555.3			552.0	547.3	543.0	537.2	532.8	527.7	516.4	502.7	488.8

<sup>a</sup> Enthalpy value on two-phase boundary.

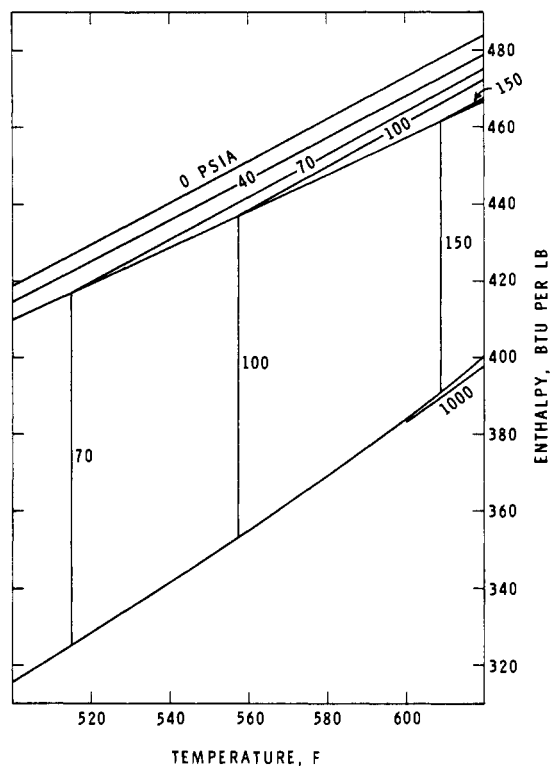


Figure 1. Enthalpy of *trans*-Decalin

liquid condition at  $75^{\circ}\text{F}$ . to the  $-200^{\circ}\text{F}$ . API data book basis.

Smoothed values of enthalpy for *cis*-Decalin are presented in Table II. Table III shows the results for *trans*-Decalin, with Figure 1 graphically showing the *trans*-Decalin results. Tables IV, V, VI, and VII show the enthalpy values for the mixtures containing, respectively, 32.2, 56.1, 72.5, and 88.4 mole % *n*-pentane. The smoothed values deviate from the measured values by an arithmetic average of 0.7 B.t.u. per pound, negligible trend, and a statistical deviation of

1.1 B.t.u. per pound. For the pure Decalins the results agree well with the results presented by Seyer (9) and McCullough *et al.* (7). The agreement is not so satisfactory compared with the results of Vvendenskii and Maioron (11). The results of Findl, Brande, and Edwards (4) on the commercial mixture of Decalins lie generally between the enthalpy values reported here for the pure isomers.

#### LITERATURE CITED

- (1) American Petroleum Institute, Division of Refining, "Technical Data Book—Petroleum Refining," Chap. 7, New York, 1966.
- (2) American Petroleum Research Project 44, "Selected Thermodynamic Properties of Hydrocarbons and Related Compounds," Texas A & M University, College Station, Tex., April 30, 1966.
- (3) Brandt, H., *Z. Physik. Chem.* **2**, 104 (1954).
- (4) Findl, E., Brande, H., Edwards, H., Study of Physicochemical Properties of Selected Military Fuels," WADD Tech. Rept. 60-767, 157-9 (December 1960).
- (5) Lenoir, J.M., Robinson, D.R., Hipkin, H.G., *J. CHEM. ENG. DATA* **15**, 23 (1970).
- (6) Lundberg, C.W., *Ibid.*, **9**, 193 (1964).
- (7) McCullough, P., Finke, H.L., Messerly, J.F., Todd, S.S., Kincheloe, T.C., Waddington, G., *J. Phys. Chem.* **61**, 1105 (1957).
- (8) Meyer, C.A., McClintock, R.B., Silvestri, A.J., Spencer, R.C., "Thermodynamic and Transport Properties of Steam," American Society of Mechanical Engineers, pp. 134-79, New York, 1967.
- (9) Seyer, W.F., *J. Amer. Chem. Soc.* **75**, 616 (1953).
- (10) Seyer, W.F., Mann, C.W., *Ibid.*, **67**, 328 (1945).
- (11) Vvendenskii, A.A., Maioron, D.M., *J. Gen. Chem. USSR* **27**, 2052 (1957).

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