

SUPPLEMENTARY MATERIAL TO
Szeged Indices of Bicyclic Graphs with Applications as
Molecular Descriptor

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Table 1: Experimental values of physical properties for 67 alkanes.

Alkanes	bp ($^{\circ}\text{C}$)	ct ($^{\circ}\text{C}$)	cp(atm)	mv(cm^3)	mr(cm^3)	hv(KJ)
Butane	-0.5	152.01	37.47			
2-methyl propane	-11.73	134.98	36			
Pentane	36.074	196.62	33.31	115.205	25.2656	26.42
2-methyl butane	27.852	187.7	32.9	116.426	25.2923	24.59
2,2 dimethylpropane	9.503	160.6	31.57	112.074	25.7243	21.78
Hexane	68.74	234.7	29.92	130.688	29.9066	31.55
2-methylpentane	60.271	224.9	29.95	131.933	29.9459	29.86
3-methylpentane	63.282	231.2	30.83	129.717	29.8016	30.27
2,2-methylbutane	49.741	216.2	30.67	132.744	29.9347	27.69
2,3-dimethylbutane	57.988	227.1	30.99	130.24	29.8104	29.12
Heptanes	98.427	267.55	27.01	146.54	34.5504	36.55
2-methylhexane	90.052	257.9	27.2	147.656	34.5908	34.8
3-methylhexane	91.85	262.4	28.1	145.821	34.4597	35.08
3-ethylpentane	93.475	267.6	28.6	143.517	34.2827	35.22
2,2-dimethylpentane	79.197	247.7	28.4	148.695	34.6166	32.43
2,3-dimethylpentane	89.784	264.6	29.2	144.153	34.3237	34.24
2,4-dimethylpentane	80.5	247.1	27.4	148.949	34.6192	32.88
3,3-dimethylpentane	86.064	263	30	144.53	34.3323	33.02
Octane	125.665	296.2	24.64	162.592	39.1922	41.48
2-methylheptane	117.647	288	24.8	163.663	39.2316	39.68
3-methylheptane	118.925	292	25.6	161.832	39.1001	39.83
4-methylheptane	117.709	290	25.6	162.105	39.1174	39.67
3-ethylhexane	118.53	292	25.74	160.07	38.94	39.4
2,2-dimethylhexane	10.84	279	25.6	164.28	39.25	37.29
2,3-dimethylhexane	115.607	293	26.6	160.39	38.98	38.79
2,4-dimethylhexane	109.42	282	25.8	163.09	39.13	37.76
2,5-dimethylhexane	109.1	279	25	164.69	39.25	37.86
3,3-dimethylhexane	111.96	290.84	27.2	160.87	39	37.93
3,4-dimethylhexane	117.72	298	27.4	158.81	38.84	39.02
3-ethyl-2-methylpentane	115.65	295	27.4	158.79	38.83	38.52
3-ethyl-3-methylpentane	118.25	305	28.9	157.02	38.71	37.99
2,2,3-trimethylpentane	109.84	294	28.2	159.52	38.92	36.91
2,2,4-trimethylpentane	99.23	271.15	25.5	165.08	39.26	35.13
2,3,3-trimethylpentane	114.76	303	29	157.29	38.76	37.22
2,3,4-trimethylpentane	113.46	295	27.6	158.85	38.86	37.61

Table 2: Experimental values of physical properties for 67 alkanes (continued).

Alkanes	bp (°C)	ct (°C)	cp(atm)	mv(cm^3)	mr(cm^3)	hv(KJ)
Nonane	150.79	322	22.74	178.71	43.84	46.44
2-methyloctane	143.26	315	23.6	179.77	43.87	44.65
3-methyloctane	144.18	318	23.7	177.95	43.72	44.75
4-methyloctane	142.48	318.3	23.06	178.15	43.76	44.75
3-ethylheptane	143	318	23.98	176.41	43.64	44.81
4-ethylheptane	141.2	318.3	23.98	175.68	43.49	44.81
2,2-dimethylheptane	132.69	302	22.8	180.5	43.91	42.28
2,3-dimethylheptane	140.5	315	23.79	176.65	43.63	43.79
2,4-dimethylheptane	133.5	306	22.7	179.12	43.73	42.87
2,5-dimethylheptane	136	307.8	22.7	179.37	43.84	43.87
2,6- dimethylheptane	135.21	306	23.7	180.91	43.92	42.82
3,3- dimethylheptane	137.3	314	24.19	176.897	43.687	42.66
3,4- dimethylheptane	140.6	322.7	24.77	175.349	43.5473	43.84
3,5- dimethylheptane	136	312.3	23.59	177.386	43.6379	42.98
4,4- dimethylheptane	135.2	317.8	24.18	176.897	43.6022	42.66
3-ethyl-2-methylhexane	138	322.7	24.77	175.445	43.655	43.84
4-ethyl-2-methylhexane	133.8	330.3	25.56	177.386	43.6472	42.98
3-ethyl-3-methylhexane	140.6	327.2	25.66	173.077	43.268	44.04
2,2,4- trimethylhexane	126.54	301	23.39	179.22	43.7638	40.57
2,2,5- trimethylhexane	124.084	296.6	22.41	181.346	43.9356	40.17
2,3,3- trimethylhexane	137.68	326.1	25.56	173.78	43.4347	42.23
2,3,4- trimethylhexane	139	324.2	25.46	173.498	43.4917	42.93
2,3,5- trimethylhexane	131.34	309.4	23.49	177.656	43.6474	41.42
3,3,4- trimethylhexane	140.46	330.6	26.45	172.055	43.3407	42.28
3,3-diethylpentane	146.168	342.8	26.94	170.185	43.1134	43.36
2,2-dimethyl-3-ethylpentane	133.83	322.6	25.96	174.537	43.4571	42.02
2,3-dimethyl-3-ethylpentane	142	338.6	26.94	170.093	42.9542	42.55
2,4-dimethyl-3-ethylpentane	136.73	324.2	25.46	173.804	43.4037	42.93
2,2,3,3-tetramethylpentane	140.274	334.5	27.04	169.495	43.2147	41
2,2,3,4- tetramethylpentane	133.016	319.6	25.66	173.557	43.4359	41
2,2,4,4- tetramethylpentane	122.284	301.6	24.58	178.256	43.8747	38.1
2,3,3,4- tetramethylpentane	141.551	334.5	26.85	169.928	43.2016	41.75

Table 3: Theoretical indices for 67 alkanes.

Alkanes	SZ^*	SZ_e^*	SZ_{ev}	SZ_{ve}
Butane	10	4.75	4	8
2-methyl propane	9	3.75	3	9
Pentane	20	11	10	20
2-methyl butane	18	9	8	22
2,2 dimethylpropane	16	7	6	24
Hexane	35	21.25	20	40
2-methylpentane	32	18.25	17	43
3-methylpentane	31	17.25	16	44
2,2-methylbutane	28	14.25	13	47
2,3-dimethylbutane	29	15.25	14	46
Heptanes	56	36.5	35	70
2-methylhexane	52	32.5	31	74
3-methylhexane	50	30.5	29	76
3-ethylpentane	48	28.5	27	78
2,2-dimethylpentane	46	26.5	25	80
2,3-dimethylpentane	46	26.5	25	80
2,4-dimethylpentane	48	28.5	27	78
3,3-dimethylpentane	44	24.5	23	82
Octane	84	57.75	56	112
2-methylheptane	79	52.75	51	117
3-methylheptane	76	49.75	48	120
4-methylheptane	75	48.75	47	121
3-ethylhexane	72	45.75	44	124
2,2-dimethylhexane	71	44.75	43	125
2,3-dimethylhexane	70	43.75	42	126
2,4-dimethylhexane	71	44.75	43	125
2,5-dimethylhexane	74	47.75	46	122
3,3-dimethylhexane	67	40.75	39	129
3,4-dimethylhexane	68	41.75	40	128
3-ethyl-2-methylpentane	67	40.75	39	129
3-ethyl-3-methylpentane	64	37.75	36	132
2,2,3-trimethylpentane	63	36.75	35	133
2,2,4-trimethylpentane	66	39.75	38	130
2,3,3-trimethylpentane	62	35.75	34	134
2,3,4-trimethylpentane	65	38.75	37	131

Table 4: Theoretical indices for 67 alkanes (continued).

Alkanes	SZ^*	SZ_e^*	SZ_{ev}	SZ_{ve}
Nonane	120	86	84	168
2-methyloctane	114	80	78	174
3-methyloctane	110	76	74	178
4-methyloctane	108	74	72	180
3-ethylheptane	104	70	68	184
4-ethylheptane	102	68	66	186
2,2-dimethylheptane	104	70	68	184
2,3-dimethylheptane	102	68	66	186
2,4-dimethylheptane	102	68	66	186
2,5-dimethylheptane	104	70	68	184
2,6- dimethylheptane	108	74	72	180
3,3- dimethylheptane	98	64	62	190
3,4- dimethylheptane	98	64	62	190
3,5- dimethylheptane	100	66	64	188
4,4- dimethylheptane	96	62	60	192
3-ethyl-2-methylhexane	96	62	60	192
4-ethyl-2-methylhexane	98	64	62	190
3-ethyl-3-methylhexane	92	58	56	196
2,2,4- trimethylhexane	94	60	58	194
2,2,5- trimethylhexane	98	64	62	190
2,3,3- trimethylhexane	90	56	54	198
2,3,4- trimethylhexane	92	58	56	196
2,3,5- trimethylhexane	96	62	60	192
3,3,4- trimethylhexane	88	54	52	200
3,3-diethylpentane	88	54	52	200
2,2-dimethyl-3-ethylpentane	88	54	52	200
2,3-dimethyl-3-ethylpentane	86	52	50	202
2,4-dimethyl-3-ethylpentane	90	56	54	198
2,2,3,3-tetramethylpentane	82	48	46	206
2,2,3,4- tetramethylpentane	86	52	50	202
2,2,4,4- tetramethylpentane	88	54	52	200
2,3,3,4- tetramethylpentane	84	50	48	204

Table 5: Theoretical distance-based indices for decane isomers.

Decanes	SZ^*	SZ_e^*	SZ_{ev}	SZ_{ve}	PI	Mo	NT
n-Decane	165	122.25	120	240	90	40	660
2-Methylnonane	158	115.25	113	247	90	42	626
3-Methylnonane	153	110.25	108	252	90	44	698
4-Methylnonane	150	107.25	105	255	90	46	764
5-Methylnonane	149	106.25	104	256	90	48	792
3-Ethyloctane	145	102.25	100	260	90	48	826
4-Ethyloctane	141	98.25	96	264	90	52	942
2,2-Dimethyloctane	146	103.25	101	259	90	46	626
2,3-Dimethyloctane	143	100.25	98	262	90	48	724
2,4-Dimethyloctane	142	99.25	97	263	90	50	754
2,5-Dimethyloctane	143	100.25	98	262	90	48	724
2,6-Dimethyloctane	146	103.25	101	259	90	46	660
2,7-Dimethyloctane	151	108.25	106	254	90	44	590
3,3-Dimethyloctane	138	95.25	93	267	90	50	794
3,4-Dimethyloctane	137	94.25	92	268	90	52	833
3,5-Dimethyloctane	138	95.25	93	267	90	50	793
3,6-Dimethyloctane	141	98.25	96	264	90	48	728
4,4-Dimethyloctane	134	91.25	89	271	90	54	906
4,5-Dimethyloctane	135	92.25	90	270	90	52	880
4-Propylheptane	138	95.25	93	267	90	54	1020
4-Isopropylheptane	131	88.25	86	274	90	56	992
3-Ethyl-2-methylheptane	134	91.25	89	271	90	54	892
4-Ethyl-2-methylheptane	134	91.25	89	271	90	54	896
5-Ethyl-2-methylheptane	138	95.25	93	267	90	50	784
3-Ethyl-3-methylheptane	129	86.25	84	276	90	56	998
4-Ethyl-3-methylheptane	129	86.25	84	276	90	56	982
3-Ethyl-5-methylheptane	133	90.25	88	272	90	52	848
3-Ethyl-4-methylheptane	130	87.25	85	275	90	54	940
4-Ethyl-4-methylheptane	126	83.25	81	279	90	58	1096
2,2,3-Trimethylheptane	130	87.25	85	275	90	54	754
2,2,4-Trimethylheptane	131	88.25	86	274	90	52	718
2,2,5-Trimethylheptane	134	91.25	89	271	90	50	652
2,2,6-Trimethylheptane	139	96.25	94	266	90	48	586
2,3,3-Trimethylheptane	127	84.25	82	278	90	56	862
2,3,4-Trimethylheptane	128	85.25	83	277	90	54	828
2,3,5-Trimethylheptane	131	88.25	86	274	90	52	746
2,3,6-Trimethylheptane	136	93.25	91	269	90	50	682
2,4,4-Trimethylheptane	127	84.25	82	278	90	56	858

Table 6: Theoretical distance-based indices for decane isomers (continued).

Decanes	SZ^*	SZ_e^*	SZ_{ev}	SZ_{ve}	PI	Mo	NT
2,4,5-Trimethylheptane	130	87.25	85	275	90	54	786
2,4,6-Trimethylheptane	135	92.25	90	270	90	52	708
2,5,5-Trimethylheptane	131	88.25	86	274	90	52	750
3,3,4-Trimethylheptane	123	80.25	78	282	90	56	906
3,3,5-Trimethylheptane	126	83.25	81	279	90	54	812
3,4,4-Trimethylheptane	122	79.25	77	283	90	58	946
3,4,5-Trimethylheptane	125	82.25	80	280	90	56	856
3-isopropyl-2-methylhexane	124	81.25	79	281	90	58	932
3,3-Diethylhexane	121	78.25	76	284	90	60	1174
3,4-Diethylhexane	125	82.25	80	280	90	56	992
3-Ethyl-2,2-dimethylhexane	122	79.25	77	283	90	58	910
4-Ethyl-2,2-dimethylhexane	126	83.25	81	279	90	54	768
3-Ethyl-2,3-dimethylhexane	119	76.25	74	286	90	60	1044
4-Ethyl-2,3-dimethylhexane	123	80.25	78	282	90	56	880
3-Ethyl-2,4-dimethylhexane	122	79.25	77	283	90	58	912
4-Ethyl-2,4-dimethylhexane	122	79.25	77	283	90	58	948
3-Ethyl-2,5-dimethylhexane	127	84.25	82	278	90	56	844
4-Ethyl-3,3-dimethylhexane	118	75.25	73	287	90	58	960
3-Ethyl-3,4-dimethylhexane	117	74.25	72	288	90	60	1024
2,2,3,3-Tetramethylhexane	115	72.25	70	290	90	60	862
2,2,3,4-Tetramethylhexane	118	75.25	73	287	90	58	768
2,2,3,5-Tetramethylhexane	123	80.25	78	282	90	56	706
2,2,4,4-Tetramethylhexane	119	76.25	74	286	90	56	730
2,2,4,5-Tetramethylhexane	124	81.25	79	281	90	54	666
2,2,5,5-Tetramethylhexane	127	84.25	82	278	90	52	574
2,3,3,4-Tetramethylhexane	115	72.25	70	290	90	60	882
2,3,3,5-Tetramethylhexane	120	77.25	75	285	90	58	812
2,3,4,4-Tetramethylhexane	116	73.25	71	289	90	58	838
2,3,4,5-Tetramethylhexane	121	78.25	76	284	90	56	768
3,3,4,4-Tetramethylhexane	111	68.25	66	294	90	60	910
3-Isopropyl-2,4-dimethylpentane	117	74.25	72	288	90	60	840
3,3-Diethyl-2-methylpentane	114	71.25	69	291	90	62	1092
3-Ethyl-2,2,3-trimethylpentane	110	67.25	65	295	90	62	928
3-Ethyl-2,2,4-trimethylpentane	115	72.25	70	290	90	60	822
3-Ethyl-2,3,4-trimethylpentane	112	69.25	67	293	90	62	960
2,2,3,3,4-Pentamethylpentane	108	65.25	63	297	90	62	780
2,2,3,4,4-Pentamethylpentane	111	68.25	66	294	90	60	672

Table 7: Theoretical degree-based indices for decane isomers.

Decanes	<i>SCI</i>	<i>R</i>	<i>RR</i>	<i>SDD</i>	M_1	M_2	F
n-Decane	4.654700538	4.914213562	16.82842712	19	34	32	66
2-Methylnonane	4.524563865	4.77005561	17.32780492	21.33333333	36	34	78
3-Methylnonane	4.549127729	4.808060412	17.45945742	20.66666667	36	35	78
4-Methylnonane	4.549127729	4.808060412	17.45945742	20.66666667	36	35	78
5-Methylnonane	4.549127729	4.808060412	17.45945742	20.66666667	36	35	78
3-Ethyloctane	4.573691594	4.846065215	17.59110992	20	36	36	78
4-Ethyloctane	4.573691594	4.846065215	17.59110992	20	36	36	78
2,2-Dimethyloctane	4.327239346	4.560660172	18.24264069	25.75	40	38	108
2,3-Dimethyloctane	4.432812155	4.680739213	18.05985573	22.66666667	38	38	90
2,4-Dimethyloctane	4.418991056	4.66390246	17.95883521	23	38	37	90
2,5-Dimethyloctane	4.418991056	4.66390246	17.95883521	23	38	37	90
2,6-Dimethyloctane	4.418991056	4.66390246	17.95883521	23	38	37	90
2,7-Dimethyloctane	4.394427191	4.625897658	17.82718272	23.66666667	38	36	90
3,3-Dimethyloctane	4.36562431	4.621320344	18.48528137	24.5	40	40	108
3,4-Dimethyloctane	4.45737602	4.718744015	18.19150823	22	38	39	90
3,5-Dimethyloctane	4.44355492	4.701907263	18.09048771	22.33333333	38	38	90
3,6-Dimethyloctane	4.44355492	4.701907263	18.09048771	22.33333333	38	38	90
4,4-Dimethyloctane	4.36562431	4.621320344	18.48528137	24.5	40	40	108
4,5-Dimethyloctane	4.45737602	4.718744015	18.19150823	22	38	39	90
4-Propylheptane	4.573691594	4.846065215	17.59110992	20	36	36	78
4-Isopropylheptane	4.45737602	4.718744015	18.19150823	22	38	39	90
3-Ethyl-2-methylheptane	4.45737602	4.718744015	18.19150823	22	38	39	90
4-Ethyl-2-methylheptane	4.44355492	4.701907263	18.09048771	22.33333333	38	38	90
5-Ethyl-2-methylheptane	4.44355492	4.701907263	18.09048771	22.33333333	38	38	90
3-Ethyl-3-methylheptane	4.404009274	4.681980515	18.72792206	23.25	40	42	108
4-Ethyl-3-methylheptane	4.481939885	4.756748817	18.32316072	21.33333333	38	40	90
3-Ethyl-5-methylheptane	4.468118785	4.739912065	18.22214021	21.66666667	38	39	90
3-Ethyl-4-methylheptane	4.481939885	4.756748817	18.32316072	21.33333333	38	40	90
4-Ethyl-4-methylheptane	4.404009274	4.681980515	18.72792206	23.25	40	42	108
2,2,3-Trimethylheptane	4.244169124	4.481380475	19.05985573	26.83333333	42	43	120
2,2,4-Trimethylheptane	4.221666537	4.454507022	18.87367098	27.41666667	42	41	120
2,2,5-Trimethylheptane	4.221666537	4.454507022	18.87367098	27.41666667	42	41	120
2,2,6-Trimethylheptane	4.197102672	4.416502219	18.74201848	28.08333333	42	40	120
2,3,3-Trimethylheptane	4.257990224	4.504035845	19.17084392	26.25	42	44	120
2,3,4-Trimethylheptane	4.341060446	4.591422815	18.79190654	24	40	42	102
2,3,5-Trimethylheptane	4.327239346	4.574586063	18.69088602	24.33333333	40	41	102
2,3,6-Trimethylheptane	4.302675481	4.53658126	18.55923352	25	40	40	102
2,4,4-Trimethylheptane	4.235487637	4.477162391	18.98465917	26.83333333	42	42	120

Table 8: Theoretical degree-based indices for decane isomers (continued).

Decanes	<i>SCI</i>	<i>R</i>	<i>RR</i>	<i>SDD</i>	M_1	M_2	<i>F</i>
2,4,5-Trimethylheptane	4.327239346	4.574586063	18.69088602	24.33333333	40	41	102
2,4,6-Trimethylheptane	4.288854382	4.519744508	18.45821301	25.33333333	40	39	102
2,5,5-Trimethylheptane	4.235487637	4.477162391	18.98465917	26.83333333	42	42	120
3,3,4-Trimethylheptane	4.282554088	4.542040647	19.30249641	25.58333333	42	45	120
3,3,5-Trimethylheptane	4.260051501	4.515167194	19.11631167	26.16666667	42	43	120
3,4,4-Trimethylheptane	4.282554088	4.542040647	19.30249641	25.58333333	42	45	120
3,4,5-Trimethylheptane	4.36562431	4.629427618	18.92355903	23.33333333	40	43	102
3-isopropyl-2-methylhexane	4.341060446	4.591422815	18.79190654	24	40	42	102
3,3-Diethylhexane	4.442394239	4.742640687	18.97056275	22	40	44	108
3,4-Diethylhexane	4.506503749	4.79475362	18.45481322	20.66666667	38	41	90
3-Ethyl-2,2-dimethylhexane	4.268732989	4.519385278	19.19150823	26.16666667	42	44	120
4-Ethyl-2,2-dimethylhexane	4.246230402	4.492511824	19.00532348	26.75	42	42	120
3-Ethyl-2,3-dimethylhexane	4.296375188	4.564696017	19.4134846	25	42	46	120
4-Ethyl-2,3-dimethylhexane	4.36562431	4.629427618	18.92355903	23.33333333	40	43	102
3-Ethyl-2,4-dimethylhexane	4.36562431	4.629427618	18.92355903	23.33333333	40	43	102
4-Ethyl-2,4-dimethylhexane	4.273872601	4.537822563	19.22729986	25.58333333	42	44	120
3-Ethyl-2,5-dimethylhexane	4.327239346	4.574586063	18.69088602	24.33333333	40	41	102
4-Ethyl-3,3-dimethylhexane	4.307117953	4.58004545	19.43414891	24.91666667	42	46	120
3-Ethyl-3,4-dimethylhexane	4.320939053	4.602700819	19.5451371	24.33333333	42	47	120
2,2,3,3-Tetramethylhexane	4.075219928	4.310660172	20.24264069	30.25	46	50	150
2,2,3,4-Tetramethylhexane	4.152417415	4.392064078	19.79190654	28.16666667	44	47	132
2,2,3,5-Tetramethylhexane	4.114032451	4.337222523	19.55923352	29.16666667	44	45	132
2,2,4,4-Tetramethylhexane	4.038163118	4.267766953	19.89949494	31.25	46	46	150
2,2,4,5-Tetramethylhexane	4.105350963	4.327185822	19.47406929	29.41666667	44	44	132
2,2,5,5-Tetramethylhexane	3.999778154	4.207106781	19.65685425	32.5	46	44	150
2,3,3,4-Tetramethylhexane	4.174920002	4.424756148	19.98805896	27.33333333	44	49	132
2,3,3,5-Tetramethylhexane	4.12785355	4.359877892	19.67022171	28.58333333	44	46	132
2,3,4,4-Tetramethylhexane	4.166238514	4.414719447	19.90289472	27.58333333	44	48	132
2,3,4,5-Tetramethylhexane	4.224744871	4.464101615	19.39230485	26	42	45	114
3,3,4,4-Tetramethylhexane	4.113604892	4.371320344	20.48528137	29	46	52	150
3-Isopropyl-2,4-dimethylpentane	4.224744871	4.464101615	19.39230485	26	42	45	114
3,3-Diethyl-2-methylpentane	4.334760152	4.625356188	19.65612529	23.75	42	48	120
3-Ethyl-2,2,3-trimethylpentane	4.113604892	4.371320344	20.48528137	29	46	52	150
3-Ethyl-2,2,4-trimethylpentane	4.152417415	4.392064078	19.79190654	28.16666667	44	47	132
3-Ethyl-2,3,4-trimethylpentane	4.188741101	4.447411518	20.09904715	26.75	44	50	132
2,2,3,3,4-Pentamethylpentane	3.967585841	4.193375673	20.92820323	32	48	54	162
2,2,3,4,4-Pentamethylpentane	3.939210519	4.154700538	20.66025404	33	48	51	162