On Molecular Polarizability: 2. Relationship to the Boiling Point of Alkanes and Alcohols

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The inner molecular polarizability index (IMPI) was developed based on the polarizability effect index (PEI). Three parameters were calculated: $N_{C(eff)}$, the quasi-length of carbon chain; ΔPEI_{OH}, the difference of polarizability effect index (PEI) of alkyl substituents in alcohols; and P_{OH}, the proportion of oxygen atom in the OH group to the total number of carbon and oxygen atoms in the alcohol. The multiple regression analysis (MRA) correlating boiling point with the three parameters was carried out for 211 alkanes and 117 alcohols. Excellent results were obtained with the correlation coefficient $r = 0.9990$ and standard deviation $s = 6.02$ °C.

1. INTRODUCTION

In part 1[1] of this work, some properties of alkanes and alcohols in solution, such as cavity surface area, water solubility, and *n*-octanol/water partition coefficients, were discussed with respect to molecular polarizability. Here we study the correlation of molecular polarizability with the boiling points of alkanes and alcohols. The relationship between the boiling point of alkanes and molecular structure had been investigated by many authors using topological indices as descriptor of molecular structure. About these works, there were some good reviews.[2,3] The relationship between the boiling point and molecular structure of alcohols was also studied with topological indices. For example, Hall et al.[4] related the boiling point of alcohols to the molecular connectivity (χ). Recently, Hall and Kier[5] set up a single-expression correlation of boiling points of alkanes and alcohols with electrotopological state indices. In it can be seen new progress in relating boiling points of organic compounds to their molecular structures quantitatively. The present paper develops an inner molecular polarizability index (IMPI) and relates the boiling points of 328 alkanes and alcohols to IMPI and polarizability effects of alkyl substituents produced by the hydroxyl group OH in alcohols.

2. INNER MOLECULAR POLARIZABLITY INDEX

In solution, the solute molecule is surrounded by solvent molecules. Thus in investigating the water solubilities of alkanes and alcohols, we put their molecules into the reaction of electric field produced by water. This is different from the pure liquid state, in which a molecule only acts against the same kind of molecule. Alkane molecules are primarily nonpolar, and their intermolecular force is dominated by dispersion force. For an alcohol molecule, the dispersion force is dominant among the alkyl parts, whereas the dipole orientation is a dominant force among the polar hydroxyl parts. Therefore, the alcohol molecule is discussed by dividing into two parts: alkyl substituent and hydroxyl group.

In a molecule of alkane, each carbon atom may be considered as connection with four substituents. If an instantaneous charge results from an outer electric field or from dispersion action forms in the *i*th carbon atom, this charge will polarize the alkyl substituents that connect with the carbon atom and make a polarizability effect PEI(*i*). Taking a sum of PEI(*i*) for all carbon atoms in a molecule of alkane, we obtained the inner molecular polarizability index (IMPI):

$$\mathrm{IMPI} = \sum \mathrm{PEI}(i) \qquad (1)$$

One should note that PEI(*i*) of this paper is different from the PEI(R_i) of part 1 of this work.[1] PEI(*i*) is the sum of the polarizability effect index of alkyl groups connected to the *i*th carbon atom, whereas PEI(R_i) is the polarizability effect index of group R_i, in which the *i*th carbon atom was taken as the beginning one in the action of the outer point charge.[1] This is why we call the ∑PEI(*i*) the inner molecular polarizability index (IMPI).

The calculation of IMPI for 2-methylbutane, for example, is described as follows:

2-methylbutane

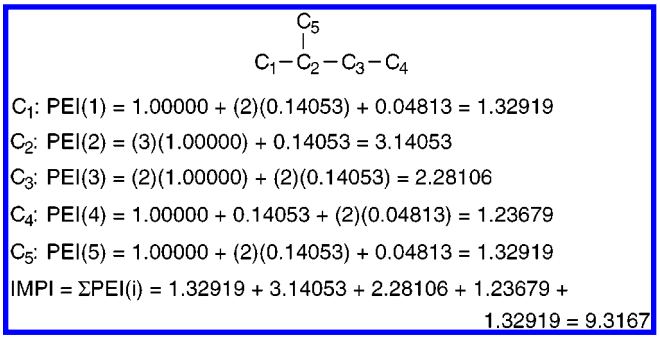

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Table 1. IMPI values of C_1-C_{10} Alkanes

no.	alkane	IMPI	no.	alkane	IMPI
1	methane	0	76	2,2,3,3,4-pentamethylpentane	23.9418
2	ethane	2	77	2,2,3,3-tetramethylhexane	23.5510
3	propane	4.2811	78	3-ethyl-2,2,3-trimethylpentane	23.7077
4	2-methylpropane	6.8432	79	3,3,4,4-tetramethylhexane	23.6883
5	butane	6.6584	80	2,2,3,4,4-pentamethylpentane	23.6530
6	2,2-dimethylpropane	9.6863	81	2,2,3,4-tetramethylhexane	23.2677
7	2-methylbutane	9.3167	82	3-ethyl-2,2,4-trimethylpentane	23.3259
8	pentane	9.0827	83	2,3,4,4-tetramethylhexane	23.3364
9	2,2-dimethylbutane	12.2562	84	2,2,3,5-tetramethylhexane	22.8580
10	2,3-dimethylbutane	12.0708	85	2,2,3-trimethylheptane	22.8096
11	2-methylpentane	11.7881	86	2,2-dimethyl-3-ethylhexane	23.1094
12	3-methylpentane	11.8373	87	3,3,4-trimethylheptane	22.9853
13	hexane	11.5348	88	3,3-dimethyl-4-ethylhexane	23.1023
14	2,2,3-trimethylbutane	15.1071	89	2,3,3,4-tetramethylhexane	23.3870
15	2,2-dimethylpentane	14.7745	90	3,4,4-trimethylheptane	23.0047
16	3,3-dimethylpentane	14.8730	91	3,4-dimethyl-3-ethylhexane	23.1516
17	2,3-dimethylpentane	14.6390	92	3-ethyl-2,3,4-trimethylpentane	23.4757
18	2,4-dimethylpentane	14.5404	93	2,3,3,5-tetramethylhexane	23.1990
19	2-methylhexane	14.2676	94	2,3,3-trimethylheptane	22.8878
20	3-methylhexane	14.3360	95	2,3-dimethyl-3-ethylhexane	23.0829
21	3-ethylpentane	14.4049	96	3,3-diethyl-2-methylpentane	23.2396
22	heptane	14.0046	97	2,2,4,4-tetramethylhexane	23.2129
23	2,2,3,3-tetramethylbutane	18.2390	98	2,2,4,5-tetramethylhexane	23.0617
24	2,2,3-trimethylpentane	17.7217	99	2,2,4-trimethylheptane	22.7305
25	2,3,3-trimethylpentane	17.8190	100	2,2-dimethyl-4-ethylhexane	22.8277
26	2,2,4-trimethylpentane	17.5739	101	3,3,5-trimethylheptane	22.8868
27	2,2-dimethylhexane	17.2816	102	2,4,4-trimethylheptane	22.8281
28	3,3-dimethylhexane	17.4189	103	2,4-dimethyl-4-ethylhexane	22.9650
29	3-ethyl-3-methylpentane	17.4369	104	2,2,5,5-tetramethylhexane	23.1391
30	2,3,4-trimethylpentane	17.4865	105	2,2,5-trimethylheptane	22.6724
31	2,3-dimethylhexane	17.1655	106	2,5,5-trimethylheptane	22.7504
32	3-ethyl-2-methylpentane	17.2536	107	2,2,6-trimethylheptane	22.5752
33	3,4-dimethylhexane	17.2342	108	2,2-dimethyloctane	22.2962
34	2,4-dimethylhexane	17.1162	109	3,3-dimethyloctane	22.4632
35	2,5-dimethylhexane	17.0282	110	4,4-dimethyloctane	22.5210
36	2-methylheptane	16.7557	111	3-ethyl-3-methylheptane	22.6537
37	3-methylheptane	16.8339	112	4-ethyl-4-methylheptane	22.7020
38	4-methylheptane	16.8533	113	3,3-diethylhexane	22.8489
39	3-ethylhexane	16.9314	114	2,3,4,5-tetramethylhexane	22.9016
40	octane	16.4874	115	2,3,4-trimethylheptane	22.5605
41	2,2,3,3-tetramethylpentane	20.9499	116	2,3-dimethyl-4-ethylhexane	22.6675
42	2,2,3,4-tetramethylpentane	20.6173	117	2,4-dimethyl-3-ethylhexane	22.6869
43	2,2,3-trimethylhexane	20.2758	118	3,4,5-trimethylheptane	22.6386
44	2,2-dimethyl-3-ethylpentane	20.5277	119	2,4-dimethyl-3-isopropylpentane	23.0920
45	3,3,4-trimethylhexane	20.4131	120	3-isopropyl-2-methylhexane	22.7309
46	2,3,3,4-tetramethylpentane	20.7172	121	2,3,5-trimethylheptane	22.5851
47	2,3,3-trimethylhexane	20.3444	122	2,5-dimethyl-3-ethylhexane	22.6429
48	2,3-dimethyl-3-ethylpentane	20.4837	123	2,4,5-trimethylheptane	22.6045
49	2,2,4,4-tetramethylpentane	20.5133	124	2,3,6-trimethylheptane	22.4780
50	2,2,4-trimethylhexane	20.1773	125	2,3-dimethyloctane	22.1949
51	2,4,4-trimethylhexane	20.2459	126	3-ethyl-2-methylheptane	22.3415
52	2,2,5-trimethylhexane	20.0698	127	3,4-dimethyloctane	22.3073
53	2,2-dimethylheptane	19.7848	128	4-isopropylheptane	22.3799
54	3,3-dimethylheptane	19.9442	129	4-ethyl-3-methylheptane	22.4005
55	4,4-dimethylheptane	19.9830	130	4,5-dimethyloctane	22.3362
56	3-ethyl-3-methylhexane	20.1104	131	3-ethyl-4-methylheptane	22.4391
57	3,3-diethylpentane	20.2477	132	3,4-diethylhexane	22.4540
58	2,3,4-trimethylhexane	19.9977	133	2,4,6-trimethylheptane	22.4676
59	2,4-dimethyl-3-ethylpentane	20.1493	134	2,4-dimethyloctane	22.1745
60	2,3,5-trimethylhexane	19.9328	135	4-ethyl-2-methylheptane	22.3018
61	2,3-dimethylheptane	19.6812	136	3,5-dimethyloctane	22.2580
62	3-ethyl-2-methylhexane	19.8076	137	3-ethyl-5-methylheptane	22.3510
63	3,4-dimethylheptane	19.7307	138	2,5-dimethyloctane	22.1551
64	3-ethyl-4-methylhexane	19.7842	139	5-ethyl-2-methylheptane	22.2440
65	2,4-dimethylheptane	19.6514	140	3,6-dimethyloctane	22.2097
66	4-ethyl-2-methylhexane	19.7390	141	2,6-dimethyloctane	22.1168
67	3,5-dimethylheptane	19.7101	142	2,7-dimethyloctane	22.0279
68	2,5-dimethylheptane	19.6126	143	2-methylnonane	21.7531
69	2,6-dimethylheptane	19.5250	144	3-methylnonane	21.8399
70	2-methyloctane	19.2513	145	4-methylnonane	21.8741
71	3-methyloctane	19.3348	146	3-ethyloctane	21.9609
72	4-methyloctane	19.3637	147	5-methylnonane	21.8836
73	3-ethylheptane	19.4472	148	4-ethyloctane	22.0046
74	4-ethylheptane	19.4760	149	4-propylheptane	22.0388
75	nonane	18.9797	150	decane	21.4794

Table 2. Boiling Point Tb and the Parameter $N_{C(eff)}$ for Alkanes

no.	compounds	$N_{C(eff)}$	Tb_{obs}[a]	Tb_{calc}[b]	$Tb_{obs} - Tb_{calc}$	no.	compounds	$N_{C(eff)}$	Tb_{obs}[a]	Tb_{calc}[b]	$Tb_{obs} - Tb_{calc}$
1	methane	1.0000	−164.00	−153.64	−10.36	71	3-methyloctane	8.8347	143.30	144.40	−1.10
2	ethane	2.0000	−88.60	−91.73	3.13	72	4-methyloctane	8.8215	142.40	144.08	−1.68
3	propane	3.0000	−42.10	−42.89	0.79	73	3-ethylheptane	8.7837	143.00	143.16	−0.16
4	2-methylpropane	3.8920	−11.70	−5.72	−5.98	74	4-ethylheptane	8.7706	141.20	142.84	−1.64
5	butane	4.0000	−0.50	−1.53	1.03	75	nonane	9.0000	150.77	148.39	2.38
6	2,2-dimethylpropane	4.6884	9.50	23.88	−14.38	76	2,2,3,3,4-pentamethylpentane	8.9715	166.05	147.71	18.34
7	2-methylbutane	4.8744	27.80	30.39	−2.59	77	2,2,3,3-tetramethylhexane	9.1204	158.00	151.26	6.74
8	pentane	5.0000	36.10	34.71	1.39	78	3-ethyl-2,2,3-trimethylpentane	9.0601	168.00	149.83	18.17
9	2,2-dimethylbutane	5.6467	49.70	56.06	−6.36	79	3,3,4,4-tetramethylhexane	9.0675	170.50	150.00	20.50
10	2,3-dimethylbutane	5.7334	58.00	58.81	−0.81	80	2,2,3,4,4-pentamethylpentane	9.0810	159.29	150.32	8.97
11	2-methylpentane	5.8710	60.30	63.13	−2.83	81	2,2,3,4-tetramethylhexane	9.2314	154.90	153.89	1.01
12	3-methylpentane	5.8465	63.30	62.37	0.93	82	3-ethyl-2,2,4-trimethylpentane	9.2084	155.30	153.35	1.95
13	hexane	6.0000	69.00	67.13	1.87	83	2,3,4,4-tetramethylhexane	9.2043	162.20	153.25	8.95
14	2,2,3-trimethylbutane	6.4892	80.90	81.86	−0.96	84	2,2,3,5-tetramethylhexane	9.3969	148.40	157.77	−9.37
15	2,2-dimethylpentane	6.6352	79.20	86.12	−6.92	85	2,2,3-trimethylheptane	9.4168	158.00	158.23	−0.23
16	3,3-dimethylpentane	6.5913	86.10	84.85	1.25	86	2,2-dimethyl-3-ethylhexane	9.2946	159.00	155.38	3.62
17	2,3-dimethylpentane	6.6967	89.80	87.90	1.90	87	3,3,4-trimethylheptane	9.3448	164.00	156.55	7.45
18	2,4-dimethylpentane	6.7420	80.50	89.21	−8.71	88	3,3-dimethyl-4-ethylhexane	9.2975	165.00	155.44	9.56
19	2-methylhexane	6.8710	90.00	92.90	−2.90	89	2,3,3,4-tetramethylhexane	9.1843	164.59	152.78	11.81
20	3-methylhexane	6.8382	92.00	91.96	0.04	90	3,4,4-trimethylh'eptane	9.3369	164.00	156.37	7.63
21	3-ethylpentane	6.8055	93.50	91.03	2.47	91	3,4-dimethyl-3-ethylhexane	9.2777	170.00	154.98	15.02
22	heptane	7.0000	98.40	96.54	1.86	92	3-ethyl-2,3,4-trimethylpentane	9.1496	169.44	151.96	17.48
23	2,2,3,3-tetramethylbutane	7.2317	106.50	102.99	3.51	93	2,3,3,5-tetramethylhexane	9.2587	153.00	154.53	−1.53
24	2,2,3-trimethylpentane	7.4428	110.00	108.75	1.25	94	2,3,3-trimethylheptane	9.3846	160.10	157.48	2.62
25	2,3,3-trimethylpentane	7.4022	114.70	107.65	7.05	95	2,3-dimethyl-3-ethylhexane	9.3053	169.00	155.63	13.37
26	2,2,4-trimethylpentane-	7.5054	99.20	110.44	−11.24	96	3,3-diethyl-2-methylpentane	9.2426	174.00	154.15	19.85
27	2,2-dimethylhexane	7.6324	106.80	113.85	−7.05	97	2,2,4,4-tetramethylhexane	9.2532	153.30	154.40	−1.10
28	3,3-dimethylhexane	7.5722	112.00	112.24	−0.24	98	2,2,4,5-tetramethylhexane	9.3139	148.20	155.83	−7.63
29	3-ethyl-2-methylpentane	7.5644	118.20	112.03	6.17	99	2,2,4-trimethylheptane	9.4496	147.70	158.99	−11.29
30	2,3,4-trimethylpentane	7.5429	113.40	111.45	1.95	100	2,2-dimethyl-4-ethylhexane	9.4094	147.00	158.06	−11.06
31	2,3-dimethylhexane	7.6840	115.60	115.22	0.38	101	3,3,5-trimethylheptane	9.3850	155.68	157.49	−1.81
32	3-ethyl-2-methylpentane	7.6448	115.60	114.18	1.42	102	2,4,4-trimethylheptane	9.4092	153.00	158.05	−5.05
33	3,4-dimethylhexane	7.6534	117.70	114.41	3.29	103	2,4-dimethyl-4-ethylhexane	9.3531	158.00	156.75	1.26
34	2,4-dimethylhexane	7.7061	109.40	115.80	−6.40	104	2,2,5,5-tetramethylhexane	9.2827	137.46	155.10	−17.64
35	2,5-dimethylhexane	7.7460	109.00	116.86	−7.86	105	2,2,5-trimethylheptane	9.4738	148.00	159.55	−11.55
36	2-methylheptane'	7.8719	117.60	120.17	−2.57	106	2,5,5-trimethylheptane	9.4413	152.80	158.80	−6.00
37	3-methylheptane	7.8353	118.00	119.21	−1.21	107	2,2,6-trimethylheptane	9.5146	148.20	160.50	−12.30
38	4-methylheptane	7.8263	117.70	118.97	−1.27	108	2,2-dimethyloctane	9.6336	155.00	163.23	−8.23
39	3-ethylhexane	7.7902	118.50	118.02	0.48	109	3,3-dimethyloctane	9.5620	161.20	161.59	−0.39
40	octane	8.0000	125.70	123.50	2.20	110	4,4-dimethyloctane	9.5375	157.50	161.03	−3.53
41	2,2,3,3-tetramethylpentane	8.1536	140.27	127.45	12.82	111	3-ethyl-3-methylheptane	9.4816	163.80	159.73	4.07
42	2,2,3,4-tetramethylpentane	8.2852	133.00	130.79	2.21	112	4-ethyl-4-methylheptane	9.4614	167.00	159.27	7.73
43	2,2,3-trimethylhexane	8.4247	131.70	134.30	−2.60	113	3,3-diethylhexane	9.4006	166.30	157.85	8.45
44	2,2-dimethyl-3-ethylpentane	8.3213	133.83	131.70	2.13	114	2,3,4,5-tetramethylhexane	9.3790	161.00	157.35	3.65
45	3,3,4-trimethylhexane	8.3676	140.50	132.87	7.63	115	2,3,4-trimethylheptane	9.5208	163.00	160.64	2.36
46	2,3,3,4-tetramethylpentane	8.2452	141.50	129.78	11.72	116	2,3-dimethyl-4-ethylhexane	9.4758	164.00	159.60	4.40
47	2,3,3-trimethylhexane	8.3963	137.70	133.59	4.11	117	2,4-dimethyl-3-ethylhexane	9.4677	164.00	159.41	4.59
48	2,3-dimethyl-3-ethylpentane	8.3392	141.60	132.15	9.45	118	3,4,5-trimethylheptane	9.4879	164.00	159.88	4.12
49	2,2,4,4-tetramethylpentane	8.3272	122.70	131.85	−9.15	119	2,4-dimethyl-3-isopropylpentane	9.3017	157.04	155.54	1.50
50	2,2,4-trimethylhexane	8.4658	126.50	135.33	−8.83	120	3-isopropyl-2-methylhexane	9.4494	163.00	158.99	4.01
51	2,4,4-trimethylhexane	8.4371	126.50	134.61	−8.11	121	2,3,5-trimethylheptane	9.5104	157.00	160.40	−3.40
52	2,2,5-trimethylhexane	8.5112	124.00	136.46	−12.46	122	2,5-dimethyl-3-ethylhexane	9.4862	157.00	159.84	−2.84
53	2,2-dimethylheptane	8.6325	132.70	139.46	−6.76	123	2,4,5-trimethylheptane	9.5023	157.00	160.21	−3.21
54	3,3-dimethylheptane	8.5684	137.30	137.88	−0.58	124	2,3,6-trimethylheptane	9.5557	155.70	161.44	−5.74
55	4,4-dimethylheptane	8.5482	135.20	137.38	−2.18	125	2,3-dimethyloctane	9.6776	164.31	164.24	0.07
56	3-ethyl-3-methylhexane	8.4940	140.60	136.03	4.57	126	3-ethyl-2-methylheptane	9.6141	166.00	162.79	3.21
57	3,3-diethylpentane	8.4364	146.20	134.59	11.61	127	3,4-dimethyloctane	9.6289	166.00	163.13	2.87
58	2,3,4-trimethylhexane	8.5419	139.00	137.22	1.78	128	4-isopropylheptane	9.5976	160.00	162.41	−2.41
59	2,4-dimethyl-3-ethylpentane	8.4776	136.73	135.62	1.11	129	4-ethyl-3-methylheptane	9.5888	167.00	162.21	4.79
60	2,3,5-trimethylhexane	8.5697	131.30	137.91	−6.61	130	4,5-dimethyloctane	9.6164	162.10	162.84	−0.74
61	2,3-dimethylheptane	8.6792	140.50	140.61	−0.11	131	3-ethyl-4-methylheptane	9.5723	167.00	161.83	5.17
62	3-ethyl-2-methylhexane	8.6238	138.00	139.25	−1.25	132	3,4-diethylhexane	9.5659	162.00	161.68	0.32
63	3,4-dimethylheptane	8.6575	140.10	140.08	0.02	133	2,4,6-trimethylheptane	9.5601	144.80	161.55	−16.75
64	3-ethyl-4-methylhexane	8.6341	140.40	139.50	0.90	134	2,4-dimethyloctane	9.6865	153.00	164.44	−11.44
65	2,4-dimethylheptane	8.6924	133.50	140.93	−7.43	135	4-ethyl-2-methylheptane	9.6312	160.00	163.18	−3.18
66	4-ethyl-2-methylhexane	8.6538	133.80	139.98	−6.18	136	3,5-dimethyloctane	9.6502	160.00	163.61	−3.61
67	3,5-dimethylheptane	8.6665	136.00	140.30	−4.30	137	3-ethyl-5-methylheptane	9.6100	158.30	162.69	−4.39
68	2,5-dimethylheptane	8.7096	136.00	141.35	−5.35	138	2,5-dimethyloctane	9.6950	156.80	164.64	−7.84
69	2,6-dimethylheptane	8.7487	135.20	142.31	−7.11	139	5-ethyl-2-methylheptane	9.6563	159.70	163.75	−4.05
70	2-methyloctane	8.8730	142.80	145.33	−2.53	140	3,6-dimethyloctane	9.6712	160.00	164.09	−4.09
141	2,6-dimethyloctane	9.7118	158.54	165.02	−6.48	177	2-methylundecane	11.8761	210.24	210.94	−0.70
142	2,7-dimethyloctane	9.7510	159.87	165.91	−6.04	178	2-methyldodecane	12.8770	229.44	230.16	−0.72

Table 2 (Continued)

no.	compounds	$N_{C(eff)}$	Tb_{obs}[a]	Tb_{calc}[b]	$Tb_{obs} - Tb_{calc}$	no.	compounds	$N_{C(eff)}$	Tb_{obs}[a]	Tb_{calc}[b]	$Tb_{obs} - Tb_{calc}$
143	2-methylnonane	9.8742	167.00	168.70	−1.70	179	2-methyltridecane	13.8777	247.44	248.29	−0.85
144	3-methylnonane	9.8349	167.80	167.81	−0.01	180	2-methyltetradecane	14.8784	264.04	265.44	−1.40
145	4-methylnonane	9.8195	165.70	167.46	−1.76	181	2-methylpentadecane	15.8790	280.84	281.71	−0.87
146	3-ethyloctane	9.7807	166.00	166.59	−0.59	182	2-methylhexadecane	16.8796	294.84	297.17	−2.33
147	5-methylnonane	9.8153	165.10	167.37	−2.27	183	2-methylheptadecane	17.8801	307.84	311.88	−4.04
148	4-ethyloctane	9.7613	163.64	166.15	−2.51	184	2-methyloctadecane	18.8805	321.84	325.91	−4.07
149	4-propylheptane	9.7462	162.00	165.80	−3.80	185	2-methylnonadecane	19.8809	333.84	339.30	−5.46
150	decane	10.0000	174.12	171.52	2.60	186	2-methyleicosane	20.8813	347.84	352.12	−4.28
151	undecane	11.0000	195.64	193.12	2.52	187	3-methyldecane	10.8355	190.84	189.67	1.17
152	dodecane	12.0000	216.14	213.38	2.76	188	3-methylundecane	11.8362	211.24	210.15	1.09
153	tridecane	13.0000	235.14	232.44	2.70	189	3-methyldodecane	12.8369	230.24	229.41	0.83
154	tetradecane	14.0000	253.54	250.44	3.10	190	3-methyltridecane	13.8376	248.44	247.58	0.86
155	pentadecane	15.0000	270.44	267.47	2.97	191	3-methyltetradecane	14.8382	265.04	264.77	0.27
156	hexadecane	16.0000	286.84	283.62	3.22	192	3-methylpentadecane	15.8389	282.04	281.07	0.97
157	heptadecane	17.0000	301.64	298.97	2.67	193	3-methylhexadecane	16.8395	294.04	296.56	−2.52
158	octadecane	18.0000	315.94	313.59	2.35	194	3-methylheptadecane	17.8400	310.04	311.30	−1.26
159	nonadecane	19.0000	328.84	327.54	1.30	195	3-methyloctadecane	18.8405	323.44	325.36	−1.92
160	eicosane	20.0000	342.84	340.86	1.98	196	3-methylnonadecane	19.8410	336.04	338.78	−2.74
161	heneicosane	21.0000	356.34	353.60	2.74	197	3-methyleicosane	20.8414	347.04	351.62	−4.58
162	docosane	22.0000	368.44	365.80	2.64	198	3-methylheneicosane	21.8416	358.04	363.91	−5.87
163	tricosane	23.0000	380.04	'377.50	2.54	199	2,3-dimethylnonane	10.6774	186.84	186.31	0.53
164	tetracosane	24.0000	391.14	388.74	2.40	200	2,3-dimethyldecane	11.6779	206.84	206.99	−0.15
165	pentacosane	25.0000	401.14	399.53	1.61	201	2,3-dimethylundecane	12.6786	226.24	226.44	−0.20
166	hexacosane	26.0000	412.04	409.90	2.14	202	2,3-dimethyldodecane	13.6795	245.84	244.78	1.06
167	heptacosnae	27.0000	421.94	419.89	2.05	203	2,3-dimethyltridecane	14.6804	263.64	262.12	1.52
168	octacosane	28.0000	431.44	429.51	1.93	204	2,3-dimethyltetradecane	15.6813	280.24	278.56	1.68
169	nonacosane	29.0000	440.64	438.78	1.86	205	2,3-dimethylpentadecane	16.6822	295.64	294.18	1.46
170	triacontane	30.0000	449.54	447.72	1.82	206	2,3-dimethylhexadecane	17.6831	310.04	309.04	1.00
171	hentriacontane	31.0000	458.54	456.36'	2.18	207	2,3-dimethylheptadecane	18.6839	324.84	323.20	1.64
172	dotriacontane	32.0000	466.94	464.69	2.25	208	2,3-dimethyloctadecane	19.6846	338.84	336.72	2.12
173	tetracontane	40.0000	525.04	522.37	2.67	209	2,3-dimethylnonadecane	20.6853	351.84	349.65	2.19
174	octacontane (n-$C_{80}H_{162}$)	80.0000	678.04	677.70	0.34	210	2,2-dimethylnonane	10.6352	177.04	185.41	−8.37
175	n-$C_{100}H_{202}$	100.0000	715.04	715.51	−0.47	211	2,2-dimethyldecane	11.6369	199.04	206.17	−7.13
176	2-methyldecane	10.8752	189.24	190.50	−1.26						

[a] Tb values (in degrees Celsius) were taken from refs 6 and 7. [b] Based on eq 8.

Values of $\Delta PEI(i)$ used in this calculation are taken from part 1 of this work.[1]

By the same calculation method, the IMPI value of *n*-pentane is 9.0827. The carbon atom numbers of 2-methylbutane and *n*-pentane are equal, while the IMPI value of 2-methylbutane is larger than that of *n*-pentane. Thus the former exhibits stronger polarization in an electric field than the latter does.

The IMPI values of alkanes bearing 1−10 carbon atoms are listed in Table 1.

For alcohols ROH, replacing OH with an H atom, we can get the IMPI value of its alkyl group by the above calculation method.

To relate directly the boiling points of alkanes and alcohols to the carbon chain length of their molecule, we now define a parameter called quasi-length of carbon chain $N_{C(eff)}$. That is, for alkane isomers bearing same carbon atom number N_C, if the inner molecule polarizability index value of the straight-chain isomer is $IMPI_{st}$ and that of a branched-chain isomer is equal to $IMPI_{br}$, then the quasi-length of carbon chain is expressed as

$$N_{C(eff)} = [IMPI_{st}/IMPI_{br}]N_C \qquad (2)$$

For example, from the IMPI values of 2-methylbutane and *n*-pentane above, we can obtain the $N_{C(eff)}$ value of 2-methylbutane to be $N_{C(eff)} = (9.0827/9.3167)(5) = 4.8744$. The calculated $N_{C(eff)}$ values of alkanes and alcohols are listed in Tables 2 and 3, respectively.

Compared with an alkane, an alcohol has a polar group OH that causes the alcohol to have a higher boiling point than the alkane. This difference is especially large for alkanes and alcohols in the lower range of molecular weight. The position of the OH group in the alcohol molecule also affects its boiling point. Thus both these factors contribute to the boiling point of alcohol. As for the effect of hydroxyl group OH position on the boiling point of the alcohol, it was counted in the difference (ΔPEI_{OH}) of polarizability effect index (PEI) of alkyl substituents in alcohols. When the alcohol has more than one hydoxyl group OH, we take the sum of ΔPEI_{OH} for all OH groups as the effect of hydroxyl group OH position on the boiling point of the alcohol. That is, the polarizability effect index value ($PEI_{R,N}$) of alkyl group R in alcohol ROH was first calculated, and then the difference of PEI was obtained:

$$\sum \Delta PEI_{OH} = \sum (PEI_{R,N} - PEI_{nor,N}) \qquad (3)$$

Here, the $PEI_{R,N}$ is the PEI of alkyl substituent bearing carbon atoms number N_C, and the $PEI_{nor,N}$ is the PEI of the corresponding straight-chain normal alkyl isomer. Taking isopropyl alcohol $(CH_3)_2CHOH$ and 1,2-propanediol CH_3-$CHOHCH_2OH$, for example, the PEI value of i-Pr is $PEI_{i-Pr,3} = 1.2811$ and the PEI value of n-Pr is $PEI_{n-Pr,3} = 1.1887$. Hence, the difference in PEI of isopropyl alcohol is

Table 3. Boiling Point Tb and Parameters $N_{C(eff)}$, $\sum\Delta PEI_{OH}$, and P_{OH} for Alcohols

no.	compounds	$N_{C(eff)}$	$\sum\Delta PEI_{OH}$	P_{OH}	Tb_{obs}[a]	Tb_{calc}[b]	$Tb_{obs} - Tb_{calc}$
212	methanol	1.0000	0.0000	0.5000	64.60	45.27	19.33
213	ethanol	2.0000	0.0000	0.3334	78.00	63.38	14.63
214	propanol	3.0000	0.0000	0.2500	97.10	85.74	11.36
215	2-propanol	3.0000	0.0924	0.2443	82.40	73.88	8.52
216	1-butanol	4.0000	0.0000	0.2000	117.60	108.86	8.74
217	2-methyl-l-propanol	3.8920	0.0246	0.1990	108.10	102.28	5.82
218	2-butanol	4.0000	0.1170	0.1955	99.50	94.81	4.69
219	2-methyl-2-propanol	3.8920	0.2094	0.1919	82.40	79.73	2.67
220	1-pentanol	5.0000	0.0000	0.1666	138.00	131.57	6.43
221	3-methyl-1-butanol	4.8744	0.0097	0.1664	131.00	126.70	4.30
222	2-methyl-l-butanol	4.8744	0.0343	0.1657	128.00	123.89	4.11
223	2-pentanol	5.0000	0.1267	0.1632	119.30	117.12	2.18
224	3-pentanol	5.0000	0.1513	0.1626	116.20	114.29	1.91
225	3-methyl-2-butanol	4.8744	0.1513	0.1626	112.90	110.42	2.48
226	2-methyl-2-butanol	4.8744	0.2437	0.1602	102.30	99.60	2.70
227	1-hexanol	6.0000	0.0000	0.1429	157.60	153.50	4.10
228	3-methyl-1-pentanol	5.8465	0.0145	0.1426	153.00	147.71	5.29
229	4-methyl-l-pentanol	5.8710	0.0048	0.1427	151.90	149.42	2.48
230	2-methyl-1-pentanol	5.8710	0.0391	0.1421	149.00	145.71	3.29
231	2-ethyl-1-butanol	5.8465	0.0488	0.1419	147.00	143.97	3.03
232	2,3-dimethyl-1-butanol	5.7334	0.0488	0.1419	144.50	140.80	3.70
233	3,3-dimethyl-1-butanol	5.6467	0.0242	0.1424	143.00	141.05	1.95
234	2-hexanol	6.0000	0.1315	0.1403	140.00	139.18	0.82
235	2,2-dimethyl-1-butanol	5.6467	0.0734	0.1647	136.50	142.16	−5.66
236	3-hexanol	6.0000	0.1658	0.1396	135.00	135.38	−0.38
237	3-methyl-2-pentanol	5.8465	0.1658	0.1396	134.30	131.06	3.24
238	4-methyl-2-pentanol	5.8710	0.1412	0.1400	131.60	134.46	−2.86
239	2-methyl-3-pentanol	5.8710	0.1905	0.1391	126.50	128.99	−2.49
240	3-methyl-3-pentanol	5.8465	0.2829	0.1373	122.40	117.88	4.52
241	2-methyl-2-pentanol	5.8710	0.2582	0.i378	121.10	121.39	−0.29
242	3,3-dimethyl-2-butanol	5.6467	0.1905	0.1391	120.40	122.54	−2.14
243	2,3-dimethyl-2-butanol	5.7334	0.2829	0.1373	118.40	114.58	3.82
244	1-heptanol	7.0000	0.0000	0.1250	176.40	174.43	1.97
245	4-methyl-1-hexanol	6.8382	0.0074	0.1249	173.00	169.58	3.42
246	5-methyl-l-hexanol	6.8710	0.0026	0.1250	170.00	170.92	−0.92
247	3-methyl-1-hexanol	6.8382	0.0236	0.1246	169.00	167.88	1.12
248	2-methyl-l-hexanol	6.8710	0.0417	0.1243	164.00	166.81	−2.81
249	2-heptanol	7.0000	0.1341	0.1229	159.00	160.40	−1.40
250	2,4-dimethyl-1-pentanol	6.7420	0.0465	0.1243	159.00	163.02	−4.02
251	3-heptanol	7.0000	0.1733	0.1224	157.00	156.27	0.73
252	4-heptanol	7.0000	0.1830	0.1222	156.00	155.23	0.77
253	5-nmethyl-2-hexanol	6.8710	0.1389	0.1229	151.00	156.59	−5.59
254	5-methyl-3-hexanol	6.8710	0.1829	0.1222	148.00	151.89	−3.89
255	2-methyl-2-hexanol	6.8710	0.2656	0.1210	143.00	142.99	0.01
256	2,3-dimethyl-2-pentanol	6.6967	0.2999	0.1205	139.70	134.60	5.10
257	2-methyl-3-hexanol	6.8710	0.2076	0.1219	143.00	149.26	−6.26
258	3-methyl-3-hexanol	6.8383	0.2999	0.1205	143.00	138.40	4.60
259	3-ethyl-3-pentanol	6.8055	0.3247	0.1201	142.00	134.80	7.20
260	2,3-dimethyl-3-pentanol	6.6967	0.3247	0.1201	139.70	131.86	7.84
261	2,4-dimethyl-3-pentanol	6.7420	0.2323	0.1215	138.70	143.18	−4.48
262	2,2-dimethyl-3-pentanol	6.6352	0.2323	0.1215	135.00	140.33	−5.33
263	2,4-dimethyl-2-pentanol	6.7420	0.2752	0.1208	133.10	138.50	−5.40
264	2,3,3-trimethyl-2-butanol	6.4892	0.3246	0.1201	131.00	126.19	4.81
265	1-octanol	8.0000	0.0000	0.1111	195.10	194.38	0.72
266	6-methyl-1-heptanol	7.8719	0.0016	0.1111	188.60	191.24	−2.64
267	4-methyl-l-heptanol	7.8268	0.0091	0.1110	188.00	189.43	−1.42
268	2-octanol	8.0000	0.1358	0.1094	180.00	180.71	−0.71
269	2,5-dimethyl-1-hexanol	7.7460	0.0460	0.1106	179.50	183.81	−4.31
270	4-octanol	8.0000	0.1920	0.1088	176.30	175.00	1.30
271	6-methyl-3-heptanol	7.8719	0.1823	0.1089	174.00	172.91	1.09
272	5-methyl-3-heptanol	7.8353	0.1920	0.1088	172.00	171.03	0.97
273	3-octanol	8.0000	0.1775	0.1090	171.00	176.49	−5.49
274	5-methyl-2-heptanol	7.8353	0.1432	0.1094	170.00	176.05	−6.05
275	4-methyl-3-heptanol	7.8268	0.2166	0.1085	170.00	168.28	1.72
276	2,4,4-trimethyl-1-pentanol	7.5054	0.0556	0.1104	168.50	177.01	−8.51
277	2-methyl-3-heptanol	7.8719	0.2166	0.1085	167.50	169.38	−1.88
278	3-methyl-2-heptanol	7.8353	0.1775	0.1090	166.10	172.53	−6.43
279	3,4-dimethyl-2-hexanol	7.6534	0.1920	0.1088	165.50	166.59	−1.09
280	2-methyl-4-heptanol	7.8719	0.2017	0.1087	164.00	170.92	−6.92
281	3-methyl-3-heptanol	7.8353	0.3090	0.1073	163.00	158.81	4.19
282	3-methyl-4-heptanol	7.8353	0.2263	0.1084	162.00	167.49	−5.49
283	4-methyl-4-heptanol	7.8263	0.3187	0.1073	161.00	157.61	3.39
284	2-methyl-3-ethyl-3-pentanol	7.5644	0.3679	0.1067	160.00	145.79	14.21
285	2,3-dimethyl-2-hexanol	7.6840	0.3090	0.1073	160.00	155.05	4.95

Table 3. Continued

no.	compounds	$N_{C(eff)}$	$\sum\Delta PEI_{OH}$	P_{OH}	Tb_{obs}[a]	Tb_{calc}[b]	$Tb_{obs} - Tb_{calc}$
286	2,3,4-trimethyl-3-pentanol	7.5429	0.3679	0.1067	156.50	145.24	11.26
287	2-methyl-3-ethyl-2-pentanol	7.5644	0.3187	0.1073	156.00	151.05	4.95
288	2-methyl-2-heptanol	7.8719	0.2699	0.1078	156.00	163.82	−7.82
289	2,5-dimethyl-2-hexanol	7.7460	0.2747	0.1078	154.50	160.24	−5.74
290	2,2,4-trimethyl-3-pentanol	7.5000	0.2756	0.1078	150.50	153.99	−3.49
291	2,2,4-trimethyl-2-pentanol	7.5054	0.3048	0.1075	147.50	151.05	−3.55
292	1-nonanol	9.0000	0.0000	0.1000	213.30	213.38	−0.08
293	7-methyl-l-octanol	8.8730	0.0011	0.1000	206.00	210.52	−4.52
294	3-nonanol	9.0000	0.1802	0.0982	195.00	195.84	−0.84
295	2-nonanol	9.0000	0.1369	0.0987	193.50	200.13	−6.63
296	5-nonanol	9.0000	0.2022	0.0980	193.00	193.68	−0.68
297	4-nonanol	9.0000	0.1974	0.0981	192.50	194.17	−1.67
298	4-ethyl-4-heptanol	8.7706	0.3632	0.0965	182.00	172.25	9.75
299	2-methyl-2-octanol	8.8730	0.2726	0.0973	178.00	183.78	−5.78
300	2,6-dimethyl-3-heptanol	8.7487	0.2268	0.0978	175.00	185.56	−10.56
301	2,6-dimethyl-4-heptanol	8.7487	0.2215	0.0978	174.50	186.08	−11.58
302	2,6-dimethyl-2-heptanol	8.7487	0.2753	0.0973	173.00	180.67	−7.67
303	3,6-dimethyl-3-heptanol	8.7096	0.3192	0.0969	173.00	175.32	−2.32
304	3,5-dimethyl-4-heptanol	8.6665	0.2708	'0.0973	187.00	179.21	7.79
305	2,2-diethyl-1-heptanol	8.4940	0.1195	0.0988	192.00	190.45	1.55
306	3,5,5-trimethyl-1-hexanol	8.4658	0.0268	0.0997	193.00	198.96	−5.96
307	2,2,3-trimethyl-3-hexanol	8.4247	0.3878	0.0963	156.00	161.54	−5.54
308	1-decanol	10.0000	0.0000	0.0909	231.10	231.46	−0.36
309	3,7-dimethyl-1-octanol	9.7118	0.0217	0.0907	212.50	223.53	−11.03
310	2-decanol	10.0000	0.1376	0.0898	211.00	218.59	−7.59
311	4-decanol	10.0000	0.2009	0.0893	210.50	212.57	−2.07
312	3,6-dimethyl-3-octanol	9.6712	0.2571	0.0888	202.20	200.15	2.05
313	3-ethyl-3-octanol	9.7807	0.3596	0.0880	199.00	192.47	6.53
314	2,6-dimethyl-4-octanol	9.7118	0.2325	0.0890	195.00	203.42	−8.42
315	2,7-dimethyl-3-octanol	9.7510	0.2282	0.0890	193.50	204.66	−11.16
316	3-ethyl-2-methyl-3-heptan'ol	9.6141	0.3988	0.0877	193.00	184.92	8.08
317	1-undecanol	11.0000	0.0000	0.0833	245.00	248.67	−3.67
318	ethylene glycol, CH_2OHCH_2OH	2.0000	0.0000	0.5000	197.20	198.75	−1.55
319	1,3-propanediol, $CH_2OHCH_2CH_2OH$	3.0000	0.0000	0.4000	214.14	207.62	6.52
320	1,2-propanediol, $CH_3CHOHCH_2OH$	3.0000	0.0924	0.3927	187.30	196.96	−9.66
321	glycerol, $CH_2OHCHOHCH_2OH$	3.0000	0.0924	0.4924	290.00	297.14	−7.14
322	1,4-butanediol, $CH_2OHCH_2CH_2CH_2OH$	4.0000	0.0000	0.3333	227.84	219.21	8.63
323	1,3-butanediol, $CH_3CHOHCH_2CH_2OH$	4.0000	0.1170	0.3270	206.84	206.54	0.30
324	1,2-butanediol, $CH_2OH(CH_2)_3CH_2OH$	4.0000	0.1170	0.3270	190.84	206.54	−15.70
325	1,5-pentanediol, $CH_2OH(CH_2)_3CH_2OH$	5.0000	0.0000	0.2857	238.84	232.16	6.68
326	2,2-dimethyl-1,3-propanediol, $CH_2OHC(CH_3)_2CH_2OH$	4.6884	0.1928	0.2780	202.84	203.83	−0.99
327	1,6-hexanediol, $CH_2OH(CH_2)_4CH_2OH$	6.0000	0.0000	0.2500	242.84	245.70	-2.86
328	2,3-dimethyl-2,3-butanediol, $(CH_3)_2COHCOH(CH_3)_2$	5.7334	0.6584	0.2310	172.84	171.07	1.77

[a] Tb values (in degrees Celsius) were taken from refs 6 and 7; for no. 318−328, these values were taken from refs 8 and 9. [b] Based on eq 8.

$\Delta PEI_{OH} = 1.2811 - 1.1887 = 0.0924$, and the difference in PEI of 1,2-propanediol is $\sum\Delta PEI_{OH} = (1.2811 - 1.1887) + (1.2811 - 1.2811) = 0.0924$. It is obvious that the ΔPEI_{OH} values are zero for straight-chain primary alcohols.

The presence of a hydroxyl group OH makes the boiling point of alcohol higher than that of alkane in the case of both bearing same carbon atom number. But, as the carbon chain of the molecule increases, this effect of hydroxyl group OH will decrease. This effect of group OH can be quantified by a parameter P_{OH}, which is the proportion of oxygen atom in the OH group to the total number of carbon and oxygen atoms in alcohol molecule. Since the position of the OH group in an alcohol molecule also produces a different effect on the boiling point, so in the calculation of the P_{OH} we must still think of the contribution of $\sum\Delta PEI_{OH}$ to the parameter P_{OH}:

$$P_{OH} = N_O/(N_C + N_O + \sum\Delta PEI_{OH}) \quad (4a)$$

In eq 4a, N_C is the carbon atom number, N_O is the oxygen atom number. For an alkane, $N_O = 0$ and $P_{OH} = 0$; for a monobasic alcohol, $N_O = 1$ and its P_{OH} is

$$P_{OH} = 1/(N_C + 1 + \sum\Delta PEI_{OH}) \quad (4b)$$

3. CORRELATION OF BOILING POINTS WITH PARAMETERS $N_{C(eff)}$, ΔPEI_{OH}, AND P_{OH} FOR ALKANE AND ALCOHOL

The multiple regression analysis between the boiling points (Tb, in degrees Celsius) and the parameters $N_{C(eff)}$, ΔPEI_{OH}, P_{OH} for the 211 alkanes and 117 alcohols (including 11 alcohols with more than one OH group) were carried out, and the regression equations are obtained as follows:

For the 211 alkanes (1−211 of Table 2)

$$\ln(810.00 - Tb) = 6.98512 - 0.113318(N_{C(eff)})^{2/3} \quad (5)$$

$$F = 120514.19 \quad s = 6.0456\ (°C) \quad r = 0.9991 \quad n = 211$$

For the 106 monobasic alcohols (212−317 of Table 3)

$$\ln(810.00 - Tb) = 6.99695 - 0.109839(N_{C(eff)})^{2/3} + 0.136252\ \Delta PEI_{OH} - 0.388658(P_{OH})^{1/2} \quad (6)$$

$$F = 1645.81 \quad s = 4.5727\ (°C) \quad r = 0.9899 \quad n = 106$$

For the 117 alcohols including more than one OH group (212−328 of Table 3), it was found that the oxygen atom number N_O also affects its boiling point:

$$\ln (810.00 - \mathrm{Tb}) = 6.94565 - 0.103936(N_{C(eff)})^{2/3} + 0.143729\sum\Delta\mathrm{PEI}_{OH} - 0.308304(N_O)^{3/4}(P_{OH})^{1/2} \quad (7)$$

$$F = 2002.51 \quad s = 5.0062\ (^\circ\mathrm{C}) \quad r = 0.9907 \quad n = 117$$

Combining eqs 5 and 7, we got the regression equation 8 for 328 compounds (in Tables 2 and 3) including 211 alkanes and 117 alcohols:

$$\ln (810.00 - \mathrm{Tb}) = 6.98375 - 0.113035(N_{C(eff)})^{2/3} + 0.155540\sum\Delta\mathrm{PEI}_{OH} - 0.326960(N_O)^{3/4}(P_{OH})^{1/2} \quad (8)$$

$$F = 55367.24 \quad s = 6.0210\ (^\circ\mathrm{C}) \quad r = 0.9990 \quad n = 328$$

4. DISCUSSION

It can be seen that the correlation with eq 8 of boiling points obtained is excellent. The correlation coefficient is $r = 0.9990$, the standard error is only $s = 6.02$ °C, and the expression is suitable to calculate the boiling point of alkanes and alcohols (including the saturated alcohols with more than one OH group) in a wider range of carbon atoms. Dearden[10] even suggested "so far as is known, no study has been published of the prediction of boiling points of heterogeneous compounds using topological indices, and it is likely that such predictions would not be particularly good". Recently Hall et al.[5] related boiling points of alkanes and monohydroxylic alcohols (245 compounds) to the electrotopological state indices (five parameters) and obtained an excellent result with correlation coefficient $r = 0.97$ and standard error $s = 8.0$ °C. In the present work, the correlation of boiling point with three parameters was carried out for 328 compounds of alkanes and alcohols based on the molecular polarizability effect, and we got a result of $r = 0.9990$ and $s = 6.02$ °C, better than Hall's results.

It can be seen from eq 8 that the $N_{C(eff)}$ increase raises the boiling point; and the larger the N_O and P_{OH} of an alcohol, the higher the boiling point compared with the alkane bearing same carbon atoms; for alcohols bearing same carbon atoms, if $\Delta\mathrm{PEI}_{OH}$ of an isomer increases, its boiling point decreases. Possibly the isomer with higher $\Delta\mathrm{PEI}_{OH}$ has a smaller dipole moment and lower intermolecular dipole orientation force and hence a lower boiling point.

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