

Predicting Boiling Points and Flash Points of Monochloroalkanes from Structure

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Table S1. Boiling Point Data for Training Set

Entry	Compound	Lit. T_B (K)	Ref	Lit. Y_{BP}	C	M	M_3	E	E_3	D	V	G	S	Pred. Y_{BP}	Pred. T_B (K)	AD
1	1-Chlorobutane	351.6	A	19.77	4	0	0	0	0	0	0	0	1.00	19.89	352.8	1.3
2	1-Chloro-3-methylbutane	372.1	H	21.67	4	1	0	0	0	0	0	0	1.56	21.77	373.2	1.1
3	1-Chloro-2-methylbutane	373.2	A	21.77	4	1	0	0	0	0	0	0	1.56	21.77	373.2	0.0
4	1-Chloropentane	381.6	A	22.59	5	0	0	0	0	0	0	0	1.00	22.67	382.3	0.8
5	1-Chloro-3,3-dimethylbutane	388.2	H	23.25	4	2	0	0	0	1	0	0	2.25	23.40	389.7	1.5
6	1-Chloro-2,2-dimethylbutane	390.2	Y	23.45	4	2	0	0	0	1	0	0	2.25	23.40	389.7	0.5
7	3-(Chloromethyl)pentane	399.2	K	24.39	4	0	0	1	0	0	0	0	2.25	24.51	400.3	1.2
8	1-Chloro-2-ethylbutane	399.2	Y	24.39	4	0	0	1	0	0	0	0	2.25	24.51	400.3	1.2
9	1-Chloro-2-methylpentane	401.2	T	24.60	5	1	0	0	0	0	0	0	1.44	24.48	400.1	1.1
10	1-Chloro-3-methylpentane	402.2	Y	24.70	5	0	1	0	0	0	0	0	1.44	24.63	401.5	0.6
11	1-Chlorohexane	408.3	A	25.36	6	0	0	0	0	0	0	0	1.00	25.45	409.1	0.8
12	1-Chloro-3-methylhexane	424.2	Y	27.13	6	1	0	0	0	0	0	0	1.36	27.22	424.9	0.8
13	1-Chloroheptane	433.6	A	28.22	7	0	0	0	0	0	0	0	1.00	28.22	433.5	0.0
14	1-Chloro-5-methylheptane	446.6	L	29.80	7	0	1	0	0	0	0	0	1.31	30.12	449.1	2.6
15	1-Chlorooctane	456.7	A	31.07	8	0	0	0	0	0	0	0	1.00	31.00	456.2	0.5
16	1-Chlorodecane	496.9	L	36.57	10	0	0	0	0	0	0	0	1.00	36.56	496.8	0.1
17	1-Chloroundecane	515.2	A	39.33	11	0	0	0	0	0	0	0	1.00	39.34	515.2	0.1
18	1-Chlorododecane	533.2	K	42.22	12	0	0	0	0	0	0	0	1.00	42.12	532.6	0.6
19	1-Chlorotetradecane	565.2	H	47.78	14	0	0	0	0	0	0	0	1.00	47.68	564.6	0.6
20	1-Chlorohexadecane	595.0	L	53.52	16	0	0	0	0	0	0	0	1.00	53.24	593.5	1.4
21	1-Chloroheptadecane	608.4	L	56.29	17	0	0	0	0	0	0	0	1.00	56.01	607.0	1.3
22	1-Chlorooctadecane	621.2	K	59.06	18	0	0	0	0	0	0	0	1.00	58.79	620.0	1.2
23	1-Chlorononadecane	634.2	C	61.98	19	0	0	0	0	0	0	0	1.00	61.57	632.4	1.8
24	3-Chloropentane	370.7	A	21.53	5	0	0	0	0	0	0	0	1.00	21.67	372.0	1.4
25	3-Chloro-2-methylpentane	390.9	L	23.53	5	1	0	0	0	0	0	0	1.44	23.48	390.4	0.4
26	2-Chloro-4-methylpentane	390.9	M	23.53	5	1	0	0	0	0	0	0	1.44	23.48	390.4	0.4
27	2-Chlorohexane	398.2	M	24.28	6	0	0	0	0	0	0	0	1.00	24.44	399.7	1.6
28	3-Chlorohexane	398.2	L	24.28	6	0	0	0	0	0	0	0	1.00	24.44	399.7	1.6
29	2-Chloro-5-methylhexane	416.3	M	26.24	6	1	0	0	0	0	0	0	1.36	26.22	416.1	0.2
30	4-Chloroheptane	417.2	J	26.34	7	0	0	0	0	0	0	0	1.00	27.22	425.0	7.8
31	3-Chloroheptane	423.2	M	27.02	7	0	0	0	0	0	0	0	1.00	27.22	425.0	1.8
32	2-Chloroheptane	423.2	M	27.02	7	0	0	0	0	0	0	0	1.00	27.22	425.0	1.8
33	3-Chlorooctane	446.5	M	29.79	8	0	0	0	0	0	0	0	1.00	30.00	448.2	1.7
34	2-Chlorononane	468.8	M	32.65	9	0	0	0	0	0	0	0	1.00	32.78	469.8	1.0
35	5-Chlorononane	470.8	Y	32.92	9	0	0	0	0	0	0	0	1.00	32.78	469.8	1.0
36	(S)-6-Chloro-2-methylnonane	484.0	M	34.72	9	1	0	0	0	0	0	0	1.23	34.22	480.3	3.6
37	2-Chlorodecane	489.9	L	35.56	10	0	0	0	0	0	0	0	1.00	35.56	489.9	0.0
38	2-Chlorododecane	529.4	L	41.59	12	0	0	0	0	0	0	0	1.00	41.12	526.4	2.9
39	5-Chlorododecane	529.4	M	41.60	12	0	0	0	0	0	0	0	1.00	41.12	526.4	2.9
40	5-Chlorotridecane	548.0	L	44.72	13	0	0	0	0	0	0	0	1.00	43.90	543.2	4.8
41	2-Chloro-2,3-dimethylbutane	385.2	K	22.95	4	2	0	0	0	0	1	0	2.25	22.95	385.1	0.1
42	3-Chloro-3-methylpentane	387.6	L	23.19	5	1	0	0	0	0	0	0	1.44	23.22	387.8	0.3
43	2-Chloro-2-methylpentane	387.6	M	23.19	5	1	0	0	0	0	0	0	1.44	23.22	387.8	0.3
44	2-Chloro-2,4-dimethylpentane	406.4	L	25.15	5	2	0	0	0	0	0	0	1.96	25.08	405.7	0.7
45	3-Chloro-3-methylhexane	408.2	Y	25.35	6	1	0	0	0	0	0	0	1.36	25.95	413.7	5.5

46	2-Chloro-2,3-dimethylpentane	413.4	Y	25.92	5	1	1	0	0	0	1	0	1.96	25.71	411.5	1.9
47	2-Chloro-2,3,3-trimethylbutane	413.4	Y	25.92	4	3	0	0	0	1	2	0	3.06	25.39	408.6	4.9
48	3-Chloro-3-ethylpentane	416.7	Y	26.28	5	0	0	0	1	0	0	0	1.96	26.16	415.5	1.1
49	2-Chloro-2,4,4-trimethylpentane	420.0	K	26.66	5	3	0	0	0	1	0	0	2.56	26.66	420.0	0.0
50	3-Chloro-2,3-dimethylhexane	430.8	M	27.89	6	2	0	0	0	0	1	0	1.78	28.23	433.6	2.9
51	3-Chloro-3-methylheptane	437.1	L	28.64	7	1	0	0	0	0	0	0	1.31	28.70	437.5	0.5
52	2-Chloro-2-methylheptane	437.1	M	28.64	7	1	0	0	0	0	0	0	1.31	28.70	437.5	0.5
53	3-Chloro-2,2,3-trimethylhexane	446.0	M	29.72	6	3	0	0	0	1	2	0	2.25	30.22	449.9	4.0
54	3-Chloro-3-ethylheptane	459.8	M	31.47	7	0	0	0	1	0	0	0	1.65	31.54	460.3	0.6
55	3-Chloro-3-methyloctane	459.8	M	31.47	8	1	0	0	0	0	0	0	1.27	31.45	459.7	0.1
56	6-Chloro-2,6-dimethyloctane	475.4	M	33.54	8	2	0	0	0	0	0	0	1.56	33.19	472.8	2.6
57	2-Chloro-2-methylnonane	481.3	M	34.35	9	1	0	0	0	0	0	0	1.23	34.22	480.3	0.9
58	3-Chloro-3-methylnonane	481.3	G	34.35	9	1	0	0	0	0	0	0	1.23	34.22	480.3	0.9
AAD = 1.44																

Table S2. Boiling Point Data for Test Set

Entry	Compound	Lit.	Ref	Lit.	C	M	M ₃	E	E ₃	D	V	G	S	Pred.	Pred.	AD
		T _B (K)		Y _{BP}										Y _{BP}	T _B (K)	
59	1-Chloro-2,3-dimethylbutane	397.2	K	24.18	4	2	0	0	0	0	1	0	2.25	24.21	397.5	0.3
60	1-Chloro-4-methylpentane	398.2	Y	24.28	5	1	0	0	0	0	0	0	1.44	24.48	400.1	1.9
61	3-(Chloromethyl)heptane	446.6	M	29.80	6	0	0	1	0	0	0	0	1.78	29.80	446.6	0.0
62	1-Chlorononane	476.7	H	33.71	9	0	0	0	0	0	0	0	1.00	33.78	477.2	0.5
63	1-Chloro-3,7-dimethyloctane	484.0	M	34.72	8	2	0	0	0	0	0	0	1.56	34.45	482.0	1.9
64	1-Chlorotridecane	550.3	M	45.12	13	0	0	0	0	0	0	0	1.00	44.90	549.0	1.3
65	1-Chloropentadecane	581.0	G	50.76	15	0	0	0	0	0	0	0	1.00	50.46	579.4	1.6
66	1-Chloroeicosane	644.4	G	64.36	20	0	0	0	0	0	0	0	1.00	64.35	644.3	0.0
67	2-Chlorobutane	341.4	A	18.88	4	0	0	0	0	0	0	0	1.00	18.89	341.4	0.0
68	2-Chloro-3-methylbutane	363.6	M	20.87	4	1	0	0	0	0	0	0	1.56	20.77	362.6	1.0
69	2-Chloropentane	372.2	H	21.68	5	0	0	0	0	0	0	0	1.00	21.67	372.0	0.1
70	3-Chloro-2,2-dimethylbutane	383.1	W	22.74	4	2	0	0	0	1	0	0	2.25	22.40	379.7	3.4
71	4-Chloro-2,2-dimethylpentane	406.4	M	25.15	5	2	0	0	0	1	0	0	1.96	25.02	405.1	1.3
72	2-Chloro-6-methylheptane	440.5	M	29.06	7	1	0	0	0	0	0	0	1.31	28.96	439.7	0.8
73	2-Chlorooctane	446.6	M	29.80	8	0	0	0	0	0	0	0	1.00	30.00	448.2	1.7
74	5-Chloroundecane	510.1	L	38.55	11	0	0	0	0	0	0	0	1.00	38.34	508.7	1.4
75	2-Chloro-2-methylbutane	358.8	A	20.42	4	1	0	0	0	0	0	0	1.56	20.51	359.7	0.9
76	3-Chloro-2,3-dimethylpentane	406.4	M	25.15	5	2	0	0	0	0	1	0	1.96	25.56	410.1	3.8
77	2-Chloro-2-methylhexane	413.2	L	25.89	6	1	0	0	0	0	0	0	1.36	25.95	413.7	0.5
78	2-Chloro-2,5-dimethylhexane	430.8	L	27.89	6	2	0	0	0	0	0	0	1.78	27.75	429.6	1.2
79	4-Chloro-4-methylheptane	437.1	M	28.64	7	1	0	0	0	0	0	0	1.31	28.70	437.5	0.5
80	3-Chloro-3-ethyl-2,2-dimethylpentane	445.0	M	29.60	5	2	0	1	0	1	2	0	3.24	30.35	451.0	6.0
81	2-Chloro-2-methyloctane	459.7	M	31.46	8	1	0	0	0	0	0	0	1.27	31.45	459.7	0.1
82	4-Chloro-4-methyloctane	459.8	M	31.47	8	1	0	0	0	0	0	0	1.27	31.45	459.7	0.1
															AAD =	1.26
For the entire data set:															AAD =	1.39

Calculation of T_{BP} for 2-chloro-2,4,4-trimethylpentane:

$$T_B(K) = -16.802 \times 26.66^{2/3} + 337.377 \times 26.66^{1/3} - 437.883 = 420.0 K$$

Table S3. Flash Point Data

All flash point (T_{FP}) and absolute deviation (AD) values have been rounded to the nearest tenth of a degree.

Entry	Compound	Pred. T_{BP}	Lit. T_{FP} (K)	Ref.	Using eqs 4 and 5.				Using eq 9.	
					Lit. N_{FP}	Pred. N_{FP}	Pred. T_{FP} (K)	AD	Pred. T_{FP} (K)	AD
1	1-Chlorobutane	19.89	262.1	L	20.6	21.4	267.6	5.5	264.4	2.4
2	1-Chloro-3-methylbutane	21.77	289.2	L	24.8	23.2	279.3	9.8	278.1	11.1
3	1-Chloro-2-methylbutane	21.77	283.0	L	23.8	23.2	279.3	3.6	278.1	4.9
4	1-Chloropentane	22.67	284.3	L	24.0	24.1	284.7	0.5	284.1	0.1
5	1-Chloro-3,3-dimethylbutane	23.40	292.2	L	25.3	24.8	289.2	3.0	288.9	3.2
6	1-Chloro-2,2-dimethylbutane	23.40	292.2	M	25.3	24.8	289.2	3.0	288.9	3.2
7	3-(Chloromethyl)pentane	24.51	298.2	M	26.3	25.9	295.7	2.5	295.9	2.3
8	1-Chloro-2-ethylbutane	24.51	298.2	L	26.3	25.9	295.7	2.5	295.9	2.3
9	1-Chloro-2-methylpentane	24.48	298.2	G	26.3	25.9	295.5	2.6	295.7	2.4
10	1-Chloro-3-methylpentane	24.63	298.2	M	26.3	26.0	296.4	1.7	296.6	1.5
11	1-Chlorohexane	25.45	299.9	M	26.6	26.8	301.2	1.3	301.5	1.7
12	1-Chloro-3-methylhexane	27.22	312.4	M	28.7	28.5	311.3	1.0	311.6	0.7
13	1-Chloroheptane	28.22	314.9	M	29.2	29.5	317.0	2.1	317.1	2.3
14	1-Chloro-5-methylheptane	30.12	325.7	L	31.0	31.4	327.4	1.8	326.9	1.2
15	1-Chlorooctane	31.00	334.2	S	32.6	32.2	332.2	1.9	331.2	2.9
16	1-Chlorodecane	36.56	356.2	S	36.6	37.6	361.4	5.3	356.1	0.1
17	1-Chloroundecane	39.34	367.6	M	38.8	40.3	375.4	7.9	367.1	0.5
18	1-Chlorododecane	42.12	377.7	M	40.8	43.1	389.1	11.5	377.3	0.3
19	1-Chlorotetradecane	47.68	403.2	L	45.9	48.5	415.5	12.4	396.0	7.1
20	1-Chlorohexadecane	53.24	411.3	L	47.6	53.9	440.9	29.6	412.6	1.3
21	1-Chloroheptadecane	56.01	418.4	L	49.1	56.6	453.2	34.8	420.3	1.9
22	1-Chlorooctadecane	58.79	457.2	M	57.5	59.3	465.3	n/a	427.5	n/a
23	1-Chlorononadecane	61.57	n/a	n/a	n/a	62.0	477.2	n/a	434.5	n/a
24	3-Chloropentane	21.67	283.0	M	23.8	23.1	278.7	4.3	277.3	5.6
25	3-Chloro-2-methylpentane	23.48	294.0	M	25.6	24.9	289.6	4.3	289.4	4.5
26	2-Chloro-4-methylpentane	23.48	294.0	M	25.6	24.9	289.6	4.3	289.4	4.5
27	2-Chlorohexane	24.44	298.2	M	26.3	25.8	295.3	2.8	295.5	2.7
28	3-Chlorohexane	24.44	298.2	L	26.3	25.8	295.3	2.8	295.5	2.7
29	2-Chloro-5-methylhexane	26.22	308.4	M	28.0	27.6	305.6	2.8	306.0	2.4
30	4-Chloroheptane	27.22	312.4	L	28.7	28.5	311.3	1.0	311.7	0.7
31	3-Chloroheptane	27.22	312.4	L	28.7	28.5	311.3	1.0	311.7	0.7
32	2-Chloroheptane	27.22	312.4	L	28.7	28.5	311.3	1.0	311.7	0.7
33	3-Chlorooctane	30.00	325.7	M	31.0	31.3	326.8	1.2	326.3	0.7
34	2-Chlorononane	32.78	338.3	M	33.3	34.0	341.8	3.5	339.6	1.4
35	5-Chlorononane	32.78	338.3	M	33.3	34.0	341.8	3.5	339.6	1.4
36	(S)-6-Chloro-2-methylnonane	34.22	346.9	G	34.9	35.4	349.3	2.5	346.1	0.8
37	2-Chlorodecane	35.56	350.2	L	35.5	36.7	356.3	6.2	351.9	1.7
38	2-Chlorododecane	41.12	372.7	L	39.8	42.1	384.2	11.6	373.7	1.1
39	5-Chlorododecane	41.12	372.6	M	39.8	42.1	384.2	11.6	373.7	1.1
40	5-Chlorotridecane	43.90	383.2	L	41.9	44.8	397.7	14.5	383.6	0.4
41	2-Chloro-2,3-dimethylbutane	22.95	288.1	M	24.6	24.4	286.4	1.6	285.9	2.1
42	3-Chloro-3-methylpentane	23.22	282.6	L	23.8	24.6	288.0	5.5	287.7	5.2
43	2-Chloro-2-methylpentane	23.22	294.0	L	25.6	24.6	288.0	5.9	287.7	6.2
44	2-Chloro-2,4-dimethylpentane	25.08	302.9	L	27.1	26.5	299.0	3.8	299.3	3.5
45	3-Chloro-3-methylhexane	25.95	306.7	M	27.7	27.3	304.1	2.6	304.5	2.2

46	2-Chloro-2,3-dimethylpentane	25.71	302.9	L	27.1	27.1	302.7	0.2	303.1	0.2
47	2-Chloro-2,3,3-trimethylbutane	25.39	297.5	L	26.2	26.8	300.8	3.4	301.2	3.7
48	3-Chloro-3-ethylpentane	26.16	306.7	G	27.7	27.5	305.3	1.4	305.7	1.0
49	2-Chloro-2,4,4-trimethylpentane	26.66	311.5	M	28.6	28.0	308.1	3.3	308.5	2.9
50	3-Chloro-2,3-dimethylhexane	28.23	316.7	M	29.5	29.5	317.0	0.4	317.2	0.5
51	3-Chloro-3-methylheptane	28.70	320.3	G	30.1	30.0	319.6	0.6	319.6	0.6
52	2-Chloro-2-methylheptane	28.70	320.3	L	30.1	30.0	319.6	0.6	319.6	0.6
53	3-Chloro-2,2,3-trimethylhexane	30.22	324.8	M	30.9	31.5	328.0	3.2	327.4	2.6
54	3-Chloro-3-ethylheptane	31.54	333.1	M	32.4	32.7	335.1	2.1	333.8	0.8
55	3-Chloro-3-methyloctane	31.45	333.1	M	32.4	32.7	334.7	1.6	333.4	0.4
56	6-Chloro-2,6-dimethyloctane	33.19	342.0	M	34.0	34.4	343.9	2.0	341.5	0.5
57	2-Chloro-2-methylnonane	34.22	345.3	M	34.6	35.4	349.3	4.1	346.1	0.8
58	3-Chloro-3-methylnonane	34.22	345.3	M	34.6	35.4	349.3	4.1	346.1	0.8
59	1-Chloro-2,3-dimethylbutane	24.21	294.0	M	25.6	25.6	293.9	0.0	294.0	0.1
60	1-Chloro-4-methylpentane	24.48	298.2	M	26.3	25.9	295.5	2.6	295.7	2.4
61	3-(Chloromethyl)heptane	29.80	325.7	M	31.0	31.1	325.7	0.0	325.3	0.4
62	1-Chlorononane	33.78	347.2	S	35.0	34.9	347.1	0.1	344.2	3.0
63	1-Chloro-3,7-dimethyloctane	34.45	346.9	G	34.9	35.6	350.6	3.7	347.1	0.3
64	1-Chlorotridecane	44.90	387.0	M	42.6	45.8	402.5	15.5	387.0	0.0
65	1-Chloropentadecane	50.46	403.8	L	46.0	51.2	428.3	24.6	404.5	0.8
66	1-Chloroeicosane	64.35	437.2	M	53.1	64.7	488.9	51.8	441.1	4.0
67	2-Chlorobutane	18.89	258.2	S	20.0	20.4	261.2	3.1	256.6	1.5
68	2-Chloro-3-methylbutane	20.77	278.6	M	23.1	22.3	273.1	5.4	271.0	7.6
69	2-Chloropentane	21.67	274.2	S	22.4	23.1	278.7	4.5	277.3	3.2
70	3-Chloro-2,2-dimethylbutane	22.40	288.1	M	24.6	23.9	283.1	4.9	282.3	5.7
71	4-Chloro-2,2-dimethylpentane	25.02	302.9	M	27.1	26.4	298.7	4.2	298.9	3.9
72	2-Chloro-6-methylheptane	28.96	322.0	M	30.4	30.2	321.1	0.9	321.0	1.0
73	2-Chlorooctane	30.00	325.7	M	31.0	31.3	326.8	1.2	326.3	0.7
74	5-Chloroundecane	38.34	361.7	L	37.7	39.4	370.4	8.8	363.2	1.6
75	2-Chloro-2-methylbutane	20.51	276.5	L	22.8	22.0	271.5	5.0	269.0	7.5
76	3-Chloro-2,3-dimethylpentane	25.56	302.9	M	27.1	26.9	301.8	1.0	302.2	0.7
77	2-Chloro-2-methylhexane	25.95	306.7	L	27.7	27.3	304.1	2.6	304.5	2.2
78	2-Chloro-2,5-dimethylhexane	27.75	316.7	L	29.5	29.1	314.3	2.3	314.6	2.1
79	4-Chloro-4-methylheptane	28.70	320.3	M	30.1	30.0	319.6	0.6	319.6	0.6
80	3-Chloro-3-ethyl-2,2-dimethylpentane	30.35	324.8	M	30.9	31.6	328.7	3.9	328.0	3.3
81	2-Chloro-2-methyloctane	31.45	333.1	M	32.4	32.7	334.7	1.6	333.4	0.3
82	4-Chloro-4-methyloctane	31.45	333.1	M	32.4	32.7	334.7	1.6	333.4	0.4
AAD =								5.2	AAD =	2.2

Calculation of T_{FP} for 2-chloro-2,4,4-trimethylpentane:

$$T_{FP} (K) = 150.5 \ln(26.66) - 185.6 = 308.5 K$$

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