

Tetraalkyl-Ammonium Bromide Training Set

Number	Cation Name	$T_{m,exp} / ^\circ\text{C}$	$T_{m,pred} / ^\circ\text{C}$ with eqn. 2
1	tributyl-(3-methylbutyl)-ammonium	17	46.5
2	butyl-dodecyl-dimethyl-ammonium	40	140.7
3	dimethyl-ditetradecyl-ammonium	50	107.4
4	dibutyl-hexadecyl-methyl-ammonium	51	95.9
5	tributyl-hexyl-ammonium	52	114.0
6	dodecyl-tripropyl-ammonium	56	101.6
7	dimethyl-octadecyl-octyl-ammonium	57	112.5
8	decyl-dimethyl-octadecyl-ammonium	60	107.4
9	dimethyl-octadecyl-tetradecyl-ammonium	62	98.7
10	dodecyl-dimethyl-octadecyl-ammonium	62	102.8
11	triheptyl-propyl-ammonium	65	93.5
12	dihexadecyl-dimethyl-ammonium	65	98.7
13	diethyl-hexadecyl-methyl-ammonium	71	119.0
14	trioctyl-propyl-ammonium	71	85.8
15	tributyl-hexadecyl-ammonium	75	83.4
16	hexadecyl-dimethyl-pentyl-ammonium	76	126.1
17	butyl-hexadecyl-dimethyl-ammonium	83	129.5
18	tetraheptyl-ammonium	90	84.3
19	didocosyl-dimethyl-ammonium	90	91.2
20	tetradodecyl-ammonium	90	79.0
21	tetraoctyl-ammonium	95	77.2
22	dodecyl-diethyl-propyl-ammonium	97	102.4
23	tetrahexyl-ammonium	100	93.7
24	tetrapentyl-ammonium	100	105.9
25	triethyl-hexyl-ammonium	105	140.3
26	triethyl-octyl-ammonium	107.5	132.5
27	diethyl-methyl-(2,4,4-trimethylpentyl)-ammonium	110	105.6
28	tetrabutyl-ammonium	120	125.6
29	triethyl-heptyl-ammonium	120	135.1
30	tributyl-methyl-ammonium	120	135.2
31	hexadecyl-tripropyl-ammonium	120	90.0
32	ethyl-methyl-bis(3-methylbutyl)-ammonium	127	94.1
33	dodecyl-triethyl-ammonium	130	124.4
34	(2-methylbutyl)-triethyl-ammonium	136	134.8
35	diicosyl-dimethyl-ammonium	137	90.1
36	hexadecyl-dimethyl-octyl-ammonium	146	118.0

37	triethyl-pentyl-ammonium	146	147.3
38	(2-isopropyl-5-methylhexyl)-trimethyl-ammonium	152	188.0
39	hexadecyl-icosyl-dimethyl-ammonium	155	92.7
40	dibutyl-dimethyl-ammonium	166	171.0
41	triethyl-hexadecyl-ammonium	175	116.8
42	triethyl-octadecyl-ammonium	180	112.8
43	trimethyl-pentyl-ammonium	180	218.2
44	heptyl-trimethyl-ammonium	184	207.7
45	hexyl-trimethyl-ammonium	186	209.6
46	dodecyl-ethyl-dimethyl-ammonium	188	149.5
47	ethyl-hexadecyl-dimethyl-ammonium	190	141.1
48	butyl-trimethyl-ammonium	195	229.4
49	(3-methylbutyl)-trimethyl-ammonium	200	218.2
50	(1-isopropyl-3-methylbutyl)-trimethyl-ammonium	203	245.0
51	trimethyl-(4-methylpentyl)-ammonium	210	178.0
52	butyl-triethyl-ammonium	210	161.8
53	(1-methylheptyl)-trimethyl-ammonium	210	205.3
54	trimethyl-octyl-ammonium	215	203.6
55	(2-methylbutyl)-trimethyl-ammonium	225	221.4
56	(2-ethyldecyl)-trimethyl-ammonium	226	138.1
57	trimethyl-nonyl-ammonium	230	202.7
58	trimethyl-propyl-ammonium	240	276.6
59	decyl-trimethyl-ammonium	240	199.1
60	trimethyl-(1-butylpentyl)-ammonium	240	208.0
61	(1-ethylpropyl)-trimethyl-ammonium	245	304.9
62	trimethyl-octadecyl-ammonium	250	174.7
63	dodecyl-trimethyl-ammonium	250	194.2
64	hexadecyl-trimethyl-ammonium	250	181.8
65	trimethyl-tetradecyl-ammonium	250	188.3
66	ethyl-diisopropyl-methyl-ammonium	250	265.4
67	triethyl-isopropyl-ammonium	264	223.0
68	tetraethyl-ammonium	270	280.0
69	diethyl-isopropyl-methyl-ammonium	277	214.4
70	tetrapropyl-ammonium	280	197.6
71	(3,3-dimethylbutyl)-trimethyl-ammonium	287	324.3
72	triethyl-methyl-ammonium	300	263.1
73	diethyl-dimethyl-ammonium	320	285.3
74	isopropyl-trimethyl-ammonium	320	369.5
75	ethyl-trimethyl-ammonium	330	323.3