

Boiling point and flash point data of selected silane and germane compounds used in the paper with the title "Quantitative Property-Property Relationships (QPPRs) and Molecular-Similarity Methods for Estimating Flash Points of Si-Organic and Ge-Organic Compounds"

Axel Drefahl
Owens Technology, Inc.
5355 Capital Court, Suite 106, Reno, NV 89502
axel@owenstechnology.com

Tables 1 and 2 contain the data for substituted germanes and substituted silanes, respectively, that have been used in the paper with the title "Quantitative Property-Property Relationships (QPPRs) and Molecular-Similarity Methods for Estimating Flash Points of Si-Organic and Ge-Organic Compounds" (<http://www.iemss.org/iemss2006>) presented in Session S7 at the "Summit on Environmental Modelling and Software" in Burlington, Vermont, U.S.A. (iEMSS, July 9-13, 2006). The data include the name of each compound, the Chemical Abstract Service Registry Number (CASRN), the chemical formula, the molecular weight (M), the flash point (T_f), and the boiling point (T_b). The given value for T_b refers to the normal boiling point (T_{nb}) unless the value is followed by "/" plus a second value which then is the reduced pressure in mmHg.

TABLE 1: Flash points and boiling points of substituted germanes

No.	Compound	CASRN	Formula	M	$T_f/^\circ\text{C}$	$T_b/^\circ\text{C}$
1	Methyltrichlorogermane	993-10-2	$\text{CH}_3\text{Cl}_3\text{Ge}$	193.98	10	110.5
2	Ethyltrichlorogermane	993-42-0	$\text{C}_2\text{H}_5\text{Cl}_3\text{Ge}$	208.01	51	144
3	Dimethyldichlorogermane	1529-48-2	$\text{C}_2\text{H}_6\text{Cl}_2\text{Ge}$	173.57	21	124
4	Allyltrichlorogermane	762-67-4	$\text{C}_3\text{H}_5\text{Cl}_3\text{Ge}$	220.02	55	155.5
5	Trimethylchlorogermane	1529-47-1	$\text{C}_3\text{H}_9\text{ClGe}$	153.15	1	102
6	Diethyldichlorogermane	13314-52-8	$\text{C}_4\text{H}_{10}\text{Cl}_2\text{Ge}$	201.62	52	175
7	Chloromethyltrimethylgermane	5830-55-7	$\text{C}_4\text{H}_{11}\text{ClGe}$	167.17	6	113
8	Tetramethylgermane	865-52-1	$\text{C}_4\text{H}_{12}\text{Ge}$	132.73	-19	43.4
9	Allyltrimethylgermane	762-66-3	$\text{C}_6\text{H}_{14}\text{Ge}$	158.77	16	101
10	Triethylchlorogermane	1067-10-3	$\text{C}_6\text{H}_{15}\text{ClGe}$	195.23	38	176
11	Phenyltrimethylgermane	1626-00-2	$\text{C}_9\text{H}_{14}\text{Ge}$	194.808	53	183
12	Diphenyldichlorogermane	1613-66-7	$\text{C}_{12}\text{H}_{10}\text{Cl}_2\text{Ge}$	297.71	160	223/12
13	Tetra-n-butylgermane	1067-42-1	$\text{C}_{16}\text{H}_{36}\text{Si}$	301.05	90	274

TABLE 2: Flash points and boiling points of substituted silanes

No.	Compound	CASRN	Formula	M	$T_f/^{\circ}\text{C}$	$T_b/^{\circ}\text{C}$
1	Methyltrichlorosilane	75-79-6	$\text{CH}_3\text{Cl}_3\text{Si}$	149.48	-15	66.4
2	Vinyltrichlorosilane	75-94-5	$\text{C}_2\text{H}_3\text{Cl}_3\text{Si}$	161.49	21	93
3	1,2-Dibromoethyltrichlorosilane	4170-50-7	$\text{C}_2\text{H}_3\text{Br}_2\text{Cl}_3\text{Si}$	321.30	65	90.5/11
4	2-Bromoethyltrichlorosilane	63802-82-4	$\text{C}_2\text{H}_4\text{BrCl}_3\text{Si}$	242.40	40	171.5
5	1-Chloroethyltrichlorosilane	7787-82-8	$\text{C}_2\text{H}_4\text{Cl}_4\text{Si}$	197.95	15	136.5
6	2-Chloroethyltrichlorosilane	6233-20-1	$\text{C}_2\text{H}_4\text{Cl}_4\text{Si}$	197.95	28	152.5
7	Ethyltrichlorosilane	115-21-9	$\text{C}_2\text{H}_5\text{Cl}_3\text{Si}$	163.51	27	100.5
8	Chloromethylmethyldichlorosilane	1558-33-14	$\text{C}_2\text{H}_5\text{Cl}_3\text{Si}$	163.51	20	121.5
9	Dimethyldichlorosilane	75-78-5	$\text{C}_2\text{H}_6\text{Cl}_2\text{Si}$	129.06	-10	70.5
10	Ethylidichlorosilane	1789-58-8	$\text{C}_2\text{H}_6\text{Cl}_2\text{Si}$	129.06	-9	75
11	Dimethylchlorosilane	1066-35-9	$\text{C}_2\text{H}_7\text{ClSi}$	94.62	-25	36
12	Allyltrichlorosilane	107-37-9	$\text{C}_3\text{H}_5\text{Cl}_3\text{Si}$	175.52	31	117.5
13	3-Bromopropyltrichlorosilane	13883-39-1	$\text{C}_3\text{H}_6\text{BrCl}_3\text{Si}$	256.43	88	85.5/16
14	Vinylmethyldichlorosilane	124-70-9	$\text{C}_3\text{H}_6\text{Cl}_2\text{Si}$	141.07	4	92.5
15	3-Chloropropyltrichlorosilane	2550-06-3	$\text{C}_3\text{H}_6\text{Cl}_4\text{Si}$	211.98	84	181.5
16	n-Propyltrichlorosilane	141-57-1	$\text{C}_3\text{H}_7\text{Cl}_3\text{Si}$	177.53	35	123.5
17	Bis(chloromethyl)methylchlorosilane	18171-56-7	$\text{C}_3\text{H}_7\text{Cl}_3\text{Si}$	177.53	42	172.5
18	Bromomethyldimethylchlorosilane	16532-02-8	$\text{C}_3\text{H}_8\text{BrClSi}$	187.54	41	130.5
19	Ethylmethyldichlorosilane	4525-44-4	$\text{C}_3\text{H}_8\text{Cl}_2\text{Si}$	143.09	2	100
20	Chloromethyldimethylchlorosilane	1719-57-9	$\text{C}_3\text{H}_8\text{Cl}_2\text{Si}$	143.09	21	115.5
21	Trimethylchlorosilane	75-77-4	$\text{C}_3\text{H}_9\text{ClSi}$	108.64	-27	57.6
22	Trimethoxychlorosilane	4668-00-2	$\text{C}_3\text{H}_9\text{ClO}_3\text{Si}$	156.64	22	112
23	Trimethoxysilane	2487-90-3	$\text{C}_3\text{H}_{10}\text{O}_3\text{Si}$	122.20	-24	86.5
24	Allylmethyldichlorosilane	1873-92-3	$\text{C}_4\text{H}_8\text{Cl}_2\text{Si}$	155.10	27	119.5
25	Vinyl dimethylchlorosilane	1719-58-0	$\text{C}_4\text{H}_9\text{ClSi}$	120.65	-5	82.5
26	3-Chloropropylmethyldichlorosilane	7787-93-1	$\text{C}_4\text{H}_9\text{Cl}_3\text{Si}$	191.56	86	69/15
27	Diethyldichlorosilane	1719-53-5	$\text{C}_4\text{H}_{10}\text{Cl}_2\text{Si}$	157.11	27	130
28	n-Propylmethyldichlorosilane	4518-94-9	$\text{C}_4\text{H}_{10}\text{Cl}_2\text{Si}$	157.11	27	125
29	Bis(chloromethyl)dimethylsilane	2917-46-6	$\text{C}_4\text{H}_{10}\text{Cl}_2\text{Si}$	157.11	46	163.5
30	Bromomethyltrimethylsilane	18243-41-9	$\text{C}_4\text{H}_{11}\text{BrSi}$	167.12	16	116.5
31	Chloromethyltrimethoxysilane	5926-26-1	$\text{C}_4\text{H}_{11}\text{ClO}_3\text{Si}$	170.67	26	156
32	Ethyl dimethylchlorosilane	6917-76-6	$\text{C}_4\text{H}_{11}\text{ClSi}$	122.67	-4	91
33	Chloromethyltrimethylsilane	2344-80-1	$\text{C}_4\text{H}_{11}\text{ClSi}$	122.67	-2	97.5
34	Dimethyldimethoxysilane	1112-39-6	$\text{C}_4\text{H}_{12}\text{O}_2\text{Si}$	120.22	-8	82
35	Methyltrimethoxysilane	1185-55-3	$\text{C}_4\text{H}_{12}\text{O}_3\text{Si}$	136.22	8	102.5
36	Tetramethylsilane	75-76-3	$\text{C}_4\text{H}_{12}\text{Si}$	88.22	-27	26.65
37	Ethyl dimethylsilane	758-21-4	$\text{C}_4\text{H}_{12}\text{Si}$	88.22	-25	45.5
38	1-Bromovinyltrimethylsilane	13683-41-5	$\text{C}_5\text{H}_{11}\text{BrSi}$	179.13	15	56/80
39	2-Bromovinyltrimethylsilane	41309-43-7	$\text{C}_5\text{H}_{11}\text{BrSi}$	179.13	15	50.5/52
40	Allyl dimethylchlorosilane	4028-23-3	$\text{C}_5\text{H}_{11}\text{ClSi}$	134.68	5	111
41	Vinyltrimethylsilane	754-05-2	$\text{C}_5\text{H}_{12}\text{Si}$	100.24	-20	55
42	3-Chloropropyl dimethylchlorosilane	10605-40-0	$\text{C}_5\text{H}_{12}\text{Cl}_2\text{Si}$	171.14	40	179
43	Acetoxytrimethylsilane	2754-27-0	$\text{C}_5\text{H}_{12}\text{O}_2\text{Si}$	132.23	4	103.5
44	Vinyltrimethoxysilane	2768-02-7	$\text{C}_5\text{H}_{12}\text{O}_3\text{Si}$	148.23	23	123
45	Allyl dimethylsilane	3937-30-2	$\text{C}_5\text{H}_{12}\text{Si}$	100.24	-20	69.5
46	Chloromethyldimethylethoxysilane	13508-53-7	$\text{C}_5\text{H}_{13}\text{ClO}_2\text{Si}$	152.70	26	132.5
47	n-Propyl dimethylchlorosilane	17477-29-1	$\text{C}_5\text{H}_{13}\text{ClSi}$	136.70	10	113.5
48	Trimethylethoxysilane	1825-62-3	$\text{C}_5\text{H}_{14}\text{OSi}$	118.25	-27	75.5
49	Ethyltrimethoxysilane	5314-55-6	$\text{C}_5\text{H}_{14}\text{O}_3\text{Si}$	150.25	27	124.5
50	Phenyltrichlorosilane	98-13-5	$\text{C}_6\text{H}_5\text{Cl}_3\text{Si}$	211.55	91	201

TABLE 2 cont'd: Flash points and boiling points of substituted silanes

No.	Compound	CASRN	Formula	M	T _f /°C	T _b /°C
51	Phenyldichlorosilane	1631-84-1	C ₆ H ₆ Cl ₂ Si	177.10	48	65.5/10
52	3-Bromo-1-(trimethylsilyl)-1-propyne	38002-45-8	C ₆ H ₁₁ BrSi	191.15	62	44.5/2
53	Cyclohexyltrichlorosilane	98-12-4	C ₆ H ₁₁ Cl ₃ Si	217.60	91	90.5/10
54	1-Trimethylsilylpropyne	6224-91-5	C ₆ H ₁₂ Si	112.25	-3	99.5
55	Allyl(chloromethyl)dimethylsilane	75422-66-1	C ₆ H ₁₃ ClSi	148.71	27	164.5/50
56	n-Hexyltrichlorosilane	928-65-4	C ₆ H ₁₃ Cl ₃ Si	219.61	85	191.5
57	n-Hexyldichlorosilane	871-64-7	C ₆ H ₁₄ Cl ₂ Si	185.16	64	173.5
58	Allyltrimethoxysilane	2551-83-9	C ₆ H ₁₄ O ₃ Si	162.26	46	147
59	Allyltrimethylsilane	762-72-1	C ₆ H ₁₄ Si	114.26	7	85.5
60	3-Bromopropyltrimethoxysilane	51826-90-5	C ₆ H ₁₅ BrO ₃ Si	243.17	82	130/45
61	Chloromethylmethyldiethoxysilane	2212-10-4	C ₆ H ₁₅ ClO ₂ Si	182.72	38	160.5
62	Triethoxychlorosilane	4667-99-6	C ₆ H ₁₅ ClO ₃ Si	198.72	47	156.5
63	3-Chloropropyltrimethoxysilane	2530-87-2	C ₆ H ₁₅ ClO ₃ Si	198.72	78	100/40
64	Triethylchlorosilane	994-30-9	C ₆ H ₁₅ ClSi	150.72	30	144.5
65	t-Butyldimethylchlorosilane	18162-48-6	C ₆ H ₁₅ ClSi	150.72	22	125
66	Dimethyldiethoxysilane	78-62-6	C ₆ H ₁₆ O ₂ Si	148.28	11	114.5
67	Triethoxysilane	998-30-1	C ₆ H ₁₆ O ₃ Si	164.28	26	131.5
68	n-Propyltrimethoxysilane	1067-25-0	C ₆ H ₁₆ O ₃ Si	164.27	34	142
69	Triethylsilane	617-86-7	C ₆ H ₁₆ Si	116.28	-3	107.5
70	t-Butyldimethylsilane	29681-57-0	C ₆ H ₁₆ Si	116.28	-11	82
71	Benzyltrichlorosilane	770-10-5	C ₇ H ₇ Cl ₃ Si	225.58	87	141/10
72	p-Tolyltrichlorosilane	701-35-9	C ₇ H ₇ Cl ₃ Si	225.58	92	219
73	Phenylmethyldichlorosilane	149-74-6	C ₇ H ₈ Cl ₂ Si	191.13	82	205.5
74	Phenylmethylchlorosilane	1631-82-9	C ₇ H ₉ ClSi	156.59	40	176.5
75	Phenylmethylsilane	766-08-5	C ₇ H ₁₀ Si	122.24	25	139.5
76	Cyclohexylmethyldichlorosilane	5578-42-7	C ₇ H ₁₄ Cl ₂ Si	197.18	66	83/15
77	Chloromethyltriethoxysilane	15267-95-5	C ₇ H ₁₇ ClO ₃ Si	212.75	47	90.5/25
78	Methyltriethoxysilane	2031-67-6	C ₇ H ₁₈ O ₃ Si	178.30	30	142
79	Phenethyltrichlorosilane	940-41-0	C ₈ H ₉ Cl ₃ Si	239.60	91	94.5/3
80	Phenylethyldichlorosilane	1125-27-5	C ₈ H ₁₀ Cl ₂ Si	205.16	92	225.5
81	p-Tolylmethyldichlorosilane	25898-37-7	C ₈ H ₁₀ Cl ₂ Si	205.16	80	163/7
82	Phenyldimethylchlorosilane	768-33-2	C ₈ H ₁₁ ClSi	170.71	61	192.5
83	Phenyldimethylsilane	766-77-8	C ₈ H ₁₂ Si	136.27	38	156.5
84	Methacryloxymethyltrimethylsilane	18269-97-1	C ₈ H ₁₆ O ₂ Si	172.30	45	98/75
85	Cyclohexyldimethylsilane	71864-47-6	C ₈ H ₁₇ ClSi	176.76	63	52.5/2
86	Vinyltriethoxysilane	78-08-0	C ₈ H ₁₈ O ₃ Si	190.31	44	160.5
87	Vinyltriethylsilane	1112-54-5	C ₈ H ₁₈ Si	142.32	25	146.5
88	Tetraethylsilane	631-36-7	C ₈ H ₂₀ Si	144.33	32	154
89	Ethyltriethoxysilane	78-07-9	C ₈ H ₂₀ O ₃ Si	192.33	40	158.5
90	Allylphenyldichlorosilane	7719-03-1	C ₉ H ₁₀ Cl ₂ Si	217.17	76	101/8
91	Phenethylmethyldichlorosilane	17146-08-6	C ₉ H ₁₂ Cl ₂ Si	219.19	80	99/6
92	Benzyl dimethylchlorosilane	1833-31-4	C ₉ H ₁₃ ClSi	184.74	73	75.5/15
93	p-Tolyldimethylchlorosilane	35239-30-6	C ₉ H ₁₃ ClSi	184.74	67	216
94	Chloromethyldimethylphenylsilane	1833-51-8	C ₉ H ₁₃ ClSi	184.73	53	106/15
95	Phenylmethyldimethoxysilane	3027-21-2	C ₉ H ₁₄ O ₂ Si	182.29	76	199.5
96	Phenyltrimethoxysilane	2996-92-1	C ₉ H ₁₄ O ₃ Si	198.29	86	211
97	Phenyltrimethylsilane	768-32-1	C ₉ H ₁₄ Si	150.30	40	169.5
98	Benzyl dimethylsilane	1631-70-5	C ₉ H ₁₄ Si	150.30	65	70/15
99	Cyclohexylmethyldimethoxysilane	17865-32-6	C ₉ H ₂₀ O ₂ Si	188.34	66	196
100	Allyltriethoxysilane	2550-04-1	C ₉ H ₂₀ O ₃ Si	204.34	47	176

TABLE 2 cont'd: Flash points and boiling points of substituted silanes

No.	Compound	CASRN	Formula	<i>M</i>	<i>T_f</i> /°C	<i>T_b</i> /°C
101	Tri- <i>n</i> -propylchlorosilane	995-25-5	C ₉ H ₂₁ ClSi	192.80	76	199.5
102	3-Chloropropyltriethoxysilane	5089-70-3	C ₉ H ₂₁ ClO ₃ Si	240.80	62	101/10
103	<i>n</i> -Propyltriethoxysilane	2550-02-9	C ₉ H ₂₂ O ₃ Si	206.36	57	179.5
104	Tri- <i>n</i> -propylsilane	998-29-8	C ₉ H ₂₂ Si	158.36	43	173
105	Phenyl dimethylacetoxysilane	17887-60-4	C ₁₀ H ₁₄ O ₂ Si	194.30	72	128/44
106	Phenethyl dimethylchlorosilane	3390-61-2	C ₁₀ H ₁₅ ClSi	198.77	70	56/0.2
107	Phenyl dimethylethoxysilane	1825-58-7	C ₁₀ H ₁₆ O ₂ Si	180.32	61	93/25
108	Benzyltrimethylsilane	770-09-2	C ₁₀ H ₁₆ Si	164.32	62	190.5
109	<i>p</i> -Tolyltrimethylsilane	3728-43-6	C ₁₀ H ₁₆ Si	164.33	46	191.5
110	Phenylmethyldiethoxysilane	775-56-4	C ₁₁ H ₁₈ O ₂ Si	210.35	89	117.5/31
111	Phenethyltrimethoxysilane	49539-88-0	C ₁₁ H ₁₈ O ₃ Si	226.35	109	95.5/2
112	Diphenyldichlorosilane	80-10-4	C ₁₂ H ₁₀ Cl ₂ Si	253.20	157	304.5
113	Diphenylchlorosilane	1631-83-0	C ₁₂ H ₁₁ ClSi	218.76	105	143/10
114	Diphenylsilane	775-12-2	C ₁₂ H ₁₂ Si	184.31	98	96/13
115	Phenyltriethoxysilane	780-69-8	C ₁₂ H ₂₀ O ₃ Si	240.37	96	112.5/10
116	Diphenylmethylchlorosilane	144-79-6	C ₁₃ H ₁₃ ClSi	232.78	141	295
117	Diphenylmethylsilane	776-76-1	C ₁₃ H ₁₄ Si	198.34	120	266.5
118	(Methacryloxymethyl)phenyl dimethylsilane	18052-92-1	C ₁₃ H ₁₈ O ₂ Si	234.37	105	106.5/1
119	Benzyltriethoxysilane	2549-99-7	C ₁₃ H ₂₂ O ₃ Si	254.40	127	148/26
120	Diphenyldimethoxysilane	6843-66-9	C ₁₄ H ₁₆ O ₂ Si	244.36	121	161/15
121	Diphenylmethylethoxysilane	1825-59-8	C ₁₅ H ₁₈ O ₂ Si	242.39	165	101/0.3
122	Diphenyldiethoxysilane	2553-19-7	C ₁₆ H ₂₀ O ₂ Si	272.42	175	167/15
123	Tetra- <i>n</i> -butylsilane	994-79-6	C ₁₆ H ₃₆ Si	256.55	75	231.5