

Hallam and Carlson  
Table S1

	2a	7a	9a	10a	19a	22a	23a	33b	35a	43a	43b	47a	47b	49b	59b	65a	67a	67c	82a	85a	85b	85f	88a	98a	
ammonium hydroxide	3	-21	32	10	1	13	-2	-9	4	-1	3	16	-8	4	5	3	16	10	2	-6	15	17	0	24	
putrescine	6	-36	26	-26	-9	12	-2	-4	0	-17	1	-9	-25	-7	2	-2	-4	6	-4	-13	24	8	-6	17	
cadaverine	1	-41	21	-17	-5	13	-7	-7	12	-10	12	-8	-16	-2	7	-1	-8	14	-2	-11	29	16	0	21	
g-butyrolactone	9	34	53	-6	-7	43	4	7	81	-12	19	6	9	-1	16	6	125	20	-7	-8	47	23	2	29	
g-hexalactone	15	-39	118	18	-2	140	12	25	171	8	30	24	-36	-1	18	18	47	40	5	-3	53	54	3	24	
g-octalactone	7	-22	26	18	2	41	3	10	36	-5	27	17	-19	-3	0	20	25	16	20	-13	174	31	-16	101	
g-decalactone	-1	-12	-1	-2	-22	16	-3	17	-3	-18	2	-3	-3	0	-4	-2	7	1	-8	-11	13	-5	7	9	
d-decalactone	0	-15	-2	-11	-23	11	-2	15	-10	-16	2	0	-4	-4	2	-5	2	0	-5	1	24	-1	-1	8	
methanoic acid	-2	-14	14	31	0	33	-8	-6	-5	-9	8	-1	-20	3	25	2	5	12	-8	-9	14	7	0	4	
acetic acid	5	-11	9	18	3	32	-1	-2	-1	0	10	2	-21	5	24	4	-5	6	10	1	27	11	-5	19	
propionic acid	1	5	20	36	5	37	-3	-9	2	-5	7	7	-22	9	24	8	49	18	7	-6	41	15	-7	11	
butyric acid	11	42	138	33	10	117	-3	-11	12	-7	20	17	-27	8	34	9	132	16	7	-10	39	21	-2	11	
pentanoic acid	7	22	19	22	30	45	2	-11	36	-5	7	14	-22	2	24	2	207	11	25	-3	30	11	-7	-9	
hexanoic acid	8	3	22	19	30	117	3	22	7	5	7	9	-24	7	29	7	20	12	19	-11	40	21	-5	13	
heptanoic acid	3	-6	3	-1	-19	12	-2	-4	11	-11	20	1	-7	-4	16	-1	1	-3	-5	1	37	5	-3	-2	
octanoic acid	-2	-7	-2	-1	-26	0	2	-13	-4	-5	10	5	-11	-1	5	-1	-9	2	-7	-5	68	7	1	-5	
nonanoic acid	-2	-10	-6	2	-19	7	-4	-2	-8	-15	6	-4	0	7	-6	-4	5	-7	1	43	5	-3	-8		
linoleic acid	-7	136	3	4	-30	3	5	-11	38	-14	34	22	-20	-1	9	8	-1	-4	-7	2	58	7	-9	-5	
isobutyric acid	-2	8	19	29	7	34	-3	-9	1	-5	10	14	-19	4	30	2	-1	13	11	-7	35	14	-4	10	
isopentanoic acid	4	-4	23	24	21	41	-4	-10	5	-12	9	11	-15	6	28	3	46	15	24	1	20	14	-3	5	
pyruvic acid	3	55	22	23	-1	35	-1	-12	5	-1	9	16	-20	1	20	8	5	11	-8	-9	23	10	3	1	
2-ethylhexanoic acid	3	1	4	5	-22	19	-2	-15	-8	-25	45	21	-16	-1	21	3	-4	8	-6	-1	99	16	-12	4	
lactic acid	2	-2	6	34	-4	36	-3	-3	9	1	6	14	-21	4	16	2	3	21	-5	-11	15	10	-3	13	
3-methylthio-1-propanol	8	29	96	5	-9	38	-2	-7	188	4	37	200	-26	-1	31	-2	51	46	30	25	46	42	2	28	
dimethyl sulfide	0	-8	19	-16	-27	13	-4	-6	-2	-19	11	-2	-8	-10	64	-6	1	2	2	-8	32	21	-6	-11	
terpinolene	-6	6	-1	-7	51	19	-3	10	7	-6	12	8	-6	2	12	-4	34	15	-5	-6	36	5	6	81	
a-pinene	-2	20	-1	-2	21	33	-3	13	28	6	4	18	-8	-4	0	1	7	14	-3	3	34	1	2	30	
b-pinene	3	-11	-6	-12	40	10	-4	10	3	10	9	-4	2	1	-4	-6	-6	6	-2	3	34	1	2	-3	
(1S)-(+)-3-carene	-1	4	1	-12	123	11	-5	5	-4	9	7	5	-2	-6	-4	-3	2	11	-5	8	16	4	4	-7	
limonene	3	4	3	-5	92	34	-4	8	51	-6	6	25	-5	5	-5	-3	2	11	2	3	47	1	2	30	
a-humulene	-1	10	-2	-9	-7	9	-3	-1	3	-11	5	6	5	0	6	-1	-2	1	10	-8	-4	19	-4	6	-2
b-myrcene	2	9	-1	-9	21	19	-4	4	0	-5	7	-2	-1	-3	-5	-1	37	12	-7	3	21	2	7	20	
(-)-trans-caryophyllene	2	4	3	-6	21	8	-5	14	14	-25	8	5	-6	-7	12	-1	-6	8	-1	1	34	5	0	-4	
p-cymene	-2	-1	-2	-8	20	18	-6	3	9	-8	2	12	-2	3	-1	-8	-2	8	-12	-1	17	4	5	-9	
geranyl acetate	2	1	-5	-8	9	1	4	0	-3	-10	10	-2	-1	-4	37	-7	7	-3	241	-1	-2	-2	1	81	
a-terpineol	2	5	7	-10	85	63	-4	10	18	1	6	12	-8	-3	-8	4	19	18	3	-12	51	-2	7	11	
geraniol	-1	1	-1	-6	2	28	-6	15	9	-16	6	1	-7	-2	1	-2	49	23	29	-4	41	1	7	89	
nerol	8	10	2	-12	22	37	-3	13	10	-7	9	0	-7	7	-8	5	14	13	1	-2	42	5	7	65	
linalool	17	31	6	-14	125	52	3	29	26	-6	1	20	-14	-8	-8	2	84	7	12	-16	51	4	-2	140	
b-citronellol	3	21	6	-10	18	25	-6	8	11	-13	7	-1	-6	-5	-2	-1	6	19	5	8	41	-5	7	50	
linalool oxide	30	-14	79	1	91	25	8	17	-5	18	14	25	-9	-12	18	3	35	22	27	9	33	44	4	36	
acetaldehyde	21	165	95	25	19	71	11	11	4	4	8	55	-38	-1	62	13	12	47	10	35	37	24	5	18	
propanal	18	-16	6	-1	-52	36	-5	3	-6	-31	15	12	-40	-8	12	-7	5	15	-15	15	52	8	-9	11	
butanal	43	54	6	-2	-38	53	-6	0	65	-11	51	20	-26	-7	9	-4	62	21	7	5	53	18	-3	26	
pentanal	22	171	24	6	-20	69	-5	3	82	-13	12	28	-22	-8	11	1	45	20	10	-2	54	26	-2	27	
hexanal	19	177	34	28	-29	139	13	-10	185	-4	44	46	-21	-4	17	13	29	15	8	20	224	43	-9	29	
E2-hexenal	17	221	38	-8	58	49	45	-8	227	41	84	37	18	6	3	-2	117	47	-6	11	145	35	-8	28	
furfural	11	176	93	34	-22	29	18	28	176	-17	34	6	-19	-4	50	-1	182	36	39	-2	61	59	-12	33	
2-propenal	14	31	3	-7	-12	32	-6	6	-9	-7	11	8	-16	-3	19	2	21	5	-5	19	36	2	4	22	
acetone	1	-10	29	0	-25	38	-7	-10	8	-16	11	3	-6	-3	130	-7	27	-5	-4	-5	28	18	-9	-1	
2-butanone	8	9	94	7	-16	84	3	7	13	-8	25	16	-15	3	144	-2	67	21	17	1	39	41	-14	4	
2-pentanone	30	2	130	19	-1	148	13	10	112	12	75	74	-31	3	60	12	70	60	32	-8	115	52	-19	11	
2-heptanone	39	-2	106	17	131	111	25	0	119	42	71	209	-10	21	25	35	170	36	32	33	190	40	19	189	
6-methyl-5-hepten-2-one	46	-24	58	8	69	85	28	-11	-12	7	46	40	6	-5	0	49	234	16	61	-7	257	34	-15	232	
2,3-butanedione	3	13	60	22	35	48	15	11	13	11	69	25	7	6	97	8	84	42	20	40	71	14	11	34	
phenethyl alcohol	2	3	17	-16	14	46	-2	29	120	28	6	9	-20	45	2	-6	236	67	25	3	20	8	4	-8	
benzyl alcohol	-4	5	30	-5	-9	40	-5	34	44	52	0	8	-21	111	14	-3	116	26	23	-4	19	25	1	1	
methyl salicylate	5	-6	13	258	1	-2	-1	-7	2	20	12	-6	6	48	-4	-13	35	-2	-5	2	-8	5	-7	8	
methyl benzoate	1	-27	43	265	-12	43	-6	-12	-14	-3	32	38	-4	19	-2	-2	208	10	31	4	29	46	-9	226	
ethyl benzoate	1	-20	29	268	-6	49	-6	-3	-16	-26	6	27	-11	-6	-5	-6	198	-4	-4	-14	14	21	-5	273	
phenethyl acetate	11	-13	18	-12	7	40	-4	0	-13	-12	2	24	-15	7	34	17	185	1	19	-8	28	7	-4	24	
benzaldehyde	5	200	57	123	-15	32	-5	-5	83	36	12	22	-18	101	6	-10	200	6	-10	7	37	49	-3	30	
phenylacetaldehyde	10	43	14	64	-30	44	1	7	-17	-6	8	27	-17	79	7	3	153	17	9	10	39	20	0	27	
acetophenone	-3	10	62	254	5	32	-6	-16	10	37	10	38	-6	79	5	12	184	35	-16	-25	22	84	-12	29	
ethyl cinnamate	-4	-6	-2	-7	21	12	-1	3	-10	-19	2	-1	-1	3	-2	2	75	-1	-1	-7	35	-11	4	7	
2-methylphenol	-11	-27	36	-17	-16	9	-8	-16	-12	77	35	-11	-27	250	3	-7	-18	57	2	-14	-14	27	31	-14	-21
4-ethyl guaiacol	-1	-10	14	2	-10	7	-9	-3	-3	-5	3	-2	-5	-2	6	-8	4	31	-7	-6	39	14	-1	1	
eugenol	4	-10	10	64	-16	7	1	-6	-7	-14	10	0	-4	-6	21	-7	7	-3	-1	-4	34	12	-3	50	
methanol	10	22	25	5	-16	55	-3	35	38	-2	14	13	-21	9	18	3	3	20	3	14	17	6	-8	5	
ethanol	4	33	21	12	-12	55	6	36	34	-7	13	9	-22	1	13	2	4	26	16	17	27	2	-12	3	
1-propanol	33	180	52	-4	10																				