

SupplementaryData_TableS3. Environmental persistence, bioaccumulation, aquatic toxicity and hazard concentration value estimations for e-cigarette e-liquid chemicals. Chemicals included in U.S. Environmental Protection Agency's Hazardous waste list and in U.S. Food and Drug Administration's Harmful and Potentially Harmful Constituents in Tobacco Products and Smoke are also identified.

Variable	Description
CASRN	CAS registry number - a unique numeric identifier that provides an unambiguous means to distinguish chemical substances
PREFERRED_NAME	Common name for the chemical
log Acute HC50 ($\mu\text{g/L}$)	Hazardous concentration value (HC50; concentration affecting 50% of aquatic species) for acute toxicity (short-term)
log Chronic HC50 ($\mu\text{g/L}$)	Hazardous concentration value (HC50; concentration affecting 50% of aquatic species) for chronic toxicity (long-term)
PBTclassification	Combined classification of persistence, bioaccumulation and toxicity. E-liquid chemicals were classified as persistent (P), bioaccumulative (B) or toxic to aquatic organisms (T). Chemicals classified as PBT, BT, and PT were selected for future detailed environmental evaluations and risk assessments. Metals and metalloids were excluded for PBT classification.
HPHC	Established list of the chemicals and chemical compounds identified by U.S. Food & Drug Administration as Harmful and Potentially Harmful Constituents in Tobacco Products and Tobacco Smoke (HPHC), including proposed additions to HPHC list. Toxicity of the chemicals include Carcinogen (CA), Respiratory Toxicant (RT), Cardiovascular Toxicant (CT), Reproductive or Developmental Toxicant (RDT), Addictive (AD)
Hazardous waste listing	U.S. Environmental protection Agency's list of hazardous constituents. The hazardous waste listing number includes acute hazardous waste (P list) and toxic waste (U list).
Cigarette butt leachate	Chemicals reported in cigarette butt leachate (from Venugopal et al. 2021) are identified by 'x'
Tobacco chemical	Chemicals reported in tobacco products (from Rodgman & Perfetti 2013) are identified by 'x'

CASRN	PREFERRED_NAME	log Acute HC50 (µg/L)	log Chronic HC50 (µg/L)	PBT classification	HPHC	Hazardous waste listing	Cigarette butt leachate	Tobacco chemical
7683-64-9	Squalene	-4.00	-5.57	PT				x
593-49-7	Heptacosane	-3.82	-5.17	T				x
55282-12-7	Octadecane, 3-ethyl-5-(2-ethylbutyl)-	-4.51	-4.59	T				
6753-98-6	alpha-Humulene	-1.89	-2.92	PBT				
106-33-2	Ethyl dodecanoate	-0.21	-1.77	T				x
1117-55-1	Hexyl octanoate	-0.21	-1.77	T				
105-90-8	Geranyl propionate	-0.25	-1.60	T				x
22485-54-7	Cetyl benzoate	-0.02	-1.47	BT				x
36431-72-8	2,6,10,10-Tetramethyl-1-oxaspiro[4.5]dec-6-ene	-0.62	-1.41	BT				x
191-24-2	Benzo(g,h,i)perylene	-0.33	-1.32	PT				x
141-14-0	Citronellyl propionate	-0.29	-1.17	T				
14905-56-7	2,6,10-Trimethyltetradecane	-0.68	-1.11	PBT				
607-91-0	Myristicin	0.49	-1.10	T				x
110-38-3	Ethyl decanoate	0.28	-1.00	T				x
35158-25-9	2-(1-Methylethyl)-5-methylhex-2-enal	0.23	-0.89	T				x
6909-30-4	trans-d-Limonene oxide	-0.52	-0.82	T				x
112-61-8	Methyl stearate	0.99	-0.72	T				x
10094-34-5	alpha,alpha-Dimethylphenethyl butyrate	-0.03	-0.64	T				
8013-90-9	4-(2,6,6-trimethylcyclohex-2-en-1-yl)but-3-en-2-one	0.08	-0.55	T				x
112-62-9	Methyl (9Z)-octadec-9-enoate	0.68	-0.54	T				x
13038-45-4		0.68	-0.54	BT				
43052-87-5	1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-butenone	0.18	-0.44	T			x	x
628-97-7	Ethyl hexadecanoate	1.15	-0.36	T				
140-26-1	Phenethyl isovalerate	0.26	-0.28	T				
106-72-9	2,6-Dimethylhept-5-enal	0.46	-0.28	T				x
18479-51-1	3,7-Dimethyloct-6-en-3-ol	0.62	-0.19	T			x	x
205-99-2	Benzo(b)fluoranthene	0.57	-0.13	PBT	CA, CT	Listed		

CASRN	PREFERRED_NAME	log Acute HC50 (µg/L)	log Chronic HC50 (µg/L)	PBT classification	HPHC	Hazardous waste listing	Cigarette butt leachate	Tobacco chemical
6728-26-3	(2E)-2-Hexenal	1.00	-0.12	T				
102-16-9	Benzyl phenylacetate	0.32	-0.08	T				
3623-51-6	dl-Neomenthol	1.15	-0.08	T				
821-55-6	2-Nonanone	4.18	0.00	T				
67-47-0	5-(Hydroxymethyl)-2-furfural	4.53	0.00	Not PBT				
501-52-0	Hydrocinnamic acid	5.09	0.00	Not PBT				x
589-18-4	4-Methylbenzyl alcohol	5.58	0.00	T				x
112-39-0	Methyl hexadecanoate	1.44	0.08	T				x
4265-25-2	2-Methyl-1-benzofuran	0.60	0.11	T				
540-18-1	n-Amyl butyrate	1.00	0.18	T				x
15679-13-7	2-Isopropyl-4-methylthiazole	1.04	0.20	T				
2445-72-9	Propanoic acid, 2-methyl-, pentyl ester	0.61	0.23	T				
34995-77-2	2-Furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-, (2R,5R)-rel-	1.15	0.28	T				
5989-33-3	2-furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-, cis-	1.15	0.28	T				
104-53-0	3-Phenylpropanal	1.04	0.30	T				
93-16-3	4-Prop-1-enylveratrole	1.53	0.34	T				
2921-88-2	Chlorpyrifos	1.05	0.36	PBT				
574-09-4	Ethanone, 2-ethoxy-1,2-diphenyl-	1.59	0.40	PT				x
60-01-5	Glycerol tributyrate	0.72	0.45	T				x
87-25-2	Ethyl anthranilate	1.26	0.45	T				
124-06-1	Ethyl tetradecanoate	1.65	0.46	T				
50-32-8	Benzo(a)pyrene	1.48	0.52	PT	CA	U022		x
122-78-1	Phenylacetaldehyde	1.30	0.54	T				
105-68-0	3-Methylbutyl propanoate	1.28	0.60	T				
87-44-5	beta-Caryophyllene	1.61	0.63	BT				
3681-82-1	trans-3-Hexenyl acetate	1.34	0.72	T				x
111-12-6	Methyl 2-octynoate	1.04	0.76	T				
489-39-4	(+)-Aromadendrene	2.18	0.76	BT				x
585-74-0	Ethanone, 1-(3-methylphenyl)-	1.32	0.83	T				

CASRN	PREFERRED_NAME	log Acute HC50 (µg/L)	log Chronic HC50 (µg/L)	PBT classification	HPHC	Hazardous waste listing	Cigarette butt leachate	Tobacco chemical
621-59-0	3-Hydroxy-4-methoxy-benzaldehyde	1.94	0.88	T				x
556-67-2	Octamethylcyclotetrasiloxane	1.90	0.90	PBT				
108-48-5	2,6-Dimethylpyridine	1.45	0.99	Not PBT				x
887407-16-1	1-Nitroso-1,2,3,6-tetrahydro-2,3'-bipyridine	0.60	1.00	PT				x
1365-19-1	Linalool oxide	1.45	1.00	T				x
409-02-9	Methyl heptenone	1.86	1.04	Not PBT				x
104-20-1	4-(4-Methoxyphenyl)-2-butanone	2.20	1.08	Not PBT				x
106-29-6	Geranyl butyrate	2.51	1.11	T				x
33467-73-1	(3Z)-Hex-3-en-1-yl formate	1.32	1.15	T				x
122-48-5	4-(4-Hydroxy-3-methoxyphenyl)-2-butanone	2.08	1.15	Not PBT				x
78-32-0	Tris(4-methylphenyl) phosphate	0.53	1.18	PBT				x
7439-97-6	Mercury & Mercury Compounds	2.26	1.26	Metals	CA, RDT	Listed		
58-08-2	Caffeine	4.59	1.29	PT				
1582-09-8	Trifluralin	2.51	1.32	PBT				x
7440-50-8	Copper	2.26	1.34	Metals				
868-57-5	Methyl 2-methylbutyrate	1.72	1.34	T				x
97-62-1	Ethyl isobutyrate	1.72	1.34	T				
15707-23-0	2-Ethyl-3-methylpyrazine	2.45	1.36	Not PBT				
2847-30-5	2-Methoxy-3-methylpyrazine	2.49	1.41	Not PBT				x
206-44-0	Fluoranthene	2.13	1.48	PT		U120		x
1139-30-6	(-)-Carophyllene oxide	6.36	1.53	PBT				x
101-86-0	2-(Phenylmethylene)octanal	2.65	1.54	T				x
84-75-3	Dihexyl phthalate	2.58	1.58	T				
7440-43-9	Cadmium	2.91	1.69	Metals	CA, RT, RDT	Listed		x
7440-41-7	Beryllium	2.70	1.70	Metals	CA	Listed		x
7440-48-4	Cobalt	3.62	1.74	Metals	CA, CT			x
140-66-9	4-(1,1,3,3-Tetramethylbutyl)phenol	2.32	1.74	T				x
141-12-8	cis-3,7-Dimethyl-2,6-octadien-1-yl acetate	2.95	1.75	T				x
94-26-8	4-Hydroxybenzoic acid butyl ester	4.03	1.77	T				x
56038-13-2	Sucralose	2.28	1.79	Not PBT				x

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123-68-2	Allyl hexanoate	2.77	1.81	T				
127-91-3	beta-Pinene	2.90	1.90	T				
7440-66-6	Zinc	3.22	1.92	Metals				x
487-19-4	Pyridine, 3-(1-methyl-1H-pyrrol-2-yl)-	3.64	1.94	PT				
105-21-5	gamma-Heptalactone	1.58	1.95	T				x
83-32-9	Acenaphthene	2.96	1.96	PT				
126-72-7	Tris(2,3-dibromopropyl) phosphate	3.00	2.00	PT		U235		
6378-65-0	Hexyl hexanoate	3.28	2.00	T				x
22839-47-0	Aspartame	3.41	2.04	Not PBT				
4674-50-4	Nootkatone	2.76	2.08	T				x
13754-86-4	1,5,6,7-Tetrahydro-4H-indol-4-one	3.89	2.08	T				
1241-94-7	2-Ethylhexyl diphenyl phosphate	2.84	2.09	PT				x
128-37-0	Butylated hydroxytoluene	3.04	2.10	PT				x
218-01-9	Chrysene	3.10	2.10	PBT	CA, CT	U050		x
85-01-8	Phenanthrene	2.67	2.12	PBT				x
85-68-7	Benzyl butyl phthalate	2.95	2.17	T		Listed		x
4680-24-4	cis-(+)-Limonene oxide	3.48	2.18	T				x
208-96-8	Acenaphthylene	3.20	2.20	T				x
928-95-0	(E)-2-Hexen-1-ol	4.32	2.20	T				x
84-69-5	Diisobutyl phthalate	3.25	2.25	T				x
7440-62-2	Vanadium	3.27	2.27	Metals				x
1825-62-3	Ethoxytrimethylsilane	3.20	2.32	T				
535-77-3	m-Cymene	2.98	2.34	T				
1072-83-9	2-Acetylpyrrole	4.34	2.34	T				
54-11-5	Nicotine	3.36	2.36	PT	RDT, AD	P075		x
2623-23-6	L-Menthyl acetate	2.93	2.36	T				x
586-62-9	Terpinolene	3.37	2.37	BT				
7440-02-0	Nickel	3.38	2.38	Metals	CA, RT	Listed		x
86-73-7	Fluorene	3.38	2.38	PT				
7440-38-2	Arsenic	3.39	2.39	Metals	CA, CT, RDT	Listed		x

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123-29-5	Ethyl nonanoate	3.52	2.40	T				
120-51-4	Benzyl benzoate	3.21	2.40	T				x
96-76-4	2,4-Di-tert-butylphenol	3.21	2.40	T				x
117-81-7	Di(2-ethylhexyl) phthalate	3.63	2.41	BT		U028		x
10484-09-0	Allyl salicylate	3.51	2.41	T				x
84-74-2	1,2-Benzenedicarboxylic acid, dibutyl ester	3.17	2.43	T		U069		x
54060-30-9	Benzenamine, 3-ethynyl-	4.23	2.43	PT				x
103-50-4	Dibenzyl ether	3.44	2.44	PT				x
23726-91-2	(E)-beta-Damascone	3.08	2.45	T				x
10032-15-2	Hexyl 2-methylbutanoate	3.56	2.46	T				x
112-31-2	Decanal	3.33	2.50	T				x
84-61-7	Dicyclohexyl phthalate	3.01	2.51	T				x
7439-92-1	Lead	3.55	2.55	Metals	CA, CT, RDT	Listed		x
127-41-3	alpha-Ionone	3.18	2.56	T				x
4437-20-1	Furan, 2,2'-[dithiobis(methylene)]bis-	3.32	2.56	PT				
138-87-4	beta-Terpineol	3.72	2.57	T				x
7440-28-0	Thallium	3.60	2.60	Metals		Listed		
494-52-0	L-3-(2'-Piperidyl)pyridine	3.30	2.60	T	AD			x
125-12-2	Isobornyl acetate	3.61	2.61	T				x
5989-27-5	D-Limonene	3.73	2.61	T				
5405-41-4	Ethyl 3-hydroxybutyrate	2.60	2.63	Not PBT				x
13674-87-8	Tris(1,3-dichloro-2-propyl) phosphate	3.65	2.67	PT			x	x
532-12-7	Myosmine	3.32	2.69	T				
141-02-6	2-Ethylhexyl fumarate	2.41	2.71	T			x	x
103-41-3	Benzyl cinnamate	3.04	2.71	T				
2743-90-0	D,L-Anatabine	3.36	2.71	T				x
102-19-2	3-Methylbutyl phenylacetate	3.75	2.72	T				
142-92-7	Hexyl acetate	3.73	2.73	T				x
106-32-1	Ethyl octanoate	3.76	2.79	T				x
2639-63-6	Hexyl butyrate	3.76	2.79	T			x	x

CASRN	PREFERRED_NAME	log Acute HC50 (µg/L)	log Chronic HC50 (µg/L)	PBT classification	HPHC	Hazardous waste listing	Cigarette butt leachate	Tobacco chemical
7429-90-5	Aluminum	3.30	2.80	Metals				x
140-67-0	Estragole	3.64	2.83	T				
99-85-4	gamma-Terpinene	3.84	2.84	T				x
25415-62-7	Butanoic acid, 3-methyl-, pentyl ester	3.80	2.85	T				x
513-08-6	Tripropyl phosphate	2.00	2.85	T				
150-84-5	Citronellyl acetate	3.85	2.85	T				x
93-08-3	2'-Acetonaphthone	3.88	2.88	T				x
57-71-6	2,3-Butanedione-2-oxime	4.11	2.89	T				x
7440-47-3	Chromium	3.89	2.89	Metals	CA, RT, RDT	Listed		x
3848-24-6	2,3-Hexanedione	3.83	2.89	Not PBT				x
14371-10-9	(2E)-3-Phenylprop-2-enal	4.00	2.89	T				x
2415-72-7	Cyclopropane, propyl-	4.08	2.89	T				x
21129-27-1	Cyclohexanol, 1-methyl-4-(1-methylethyl)-	3.72	2.90	T			x	x
104-46-1	Anethole	4.11	2.90	T				x
659-70-1	3-Methylbutyl 3-methylbutanoate	3.84	2.91	T				
91-64-5	Coumarin	3.92	2.92	T	Banned in food		x	x
89-79-2	(-)-Isopulegol	4.62	2.92	T			x	x
119-61-9	Benzophenone	3.55	2.93	T				
1504-74-1	2'-Methoxycinnamaldehyde	4.08	2.93	T			x	x
80-56-8	alpha-Pinene	3.94	2.94	BT				
115-86-6	Triphenyl phosphate	3.17	2.94	PT				
89-83-8	Thymol	3.94	2.94	T				
61683-99-6	1,3-Benzodioxole, 5-(4-methyl-1,3-dioxolan-2-yl)-	4.90	2.95	T				x
562-74-3	4-Methyl-1-(propan-2-yl)cyclohex-3-en-1-ol	5.94	2.96	T			x	x
94-86-0	2-Ethoxy-5-(1-propenyl)phenol	3.48	2.97	T			x	x
22438-36-4	Butane, 2-[[1-methylethylthio]-	3.81	2.98	PT			x	x
108-38-3	m-Xylene	3.99	2.99	T				x
103-54-8	3-Phenylprop-2-en-1-yl acetate	3.97	3.00	T				x
79-77-6	beta-Ionone	3.85	3.02	T				x

CASRN	PREFERRED_NAME	log Acute HC50 (µg/L)	log Chronic HC50 (µg/L)	PBT classification	HPHC	Hazardous waste listing	Cigarette butt leachate	Tobacco chemical
94-13-3	Propylparaben	4.03	3.03	T			x	x
7440-31-5	Tin	4.03	3.03	Metals				x
95-47-6	o-Xylene	4.04	3.04	T				x
120-57-0	Piperonal	4.11	3.04	T				x
141-27-5	(2E)-3,7-dimethylocta-2,6-dienal	4.23	3.05	T				x
5392-40-5	3,7-Dimethyl-2,6-octadienal	4.65	3.05	T				x
24851-98-7	Methyl dihydrojasmonate	4.30	3.06	T				x
103-26-4	Methyl cinnamate	3.87	3.07	T				x
2305-05-7	gamma-Dodecalactone	3.40	3.08	T				x
106-42-3	p-Xylene	3.96	3.08	T				x
99-86-5	alpha-Terpinene	3.87	3.08	T				x
470-67-7	1,4-Cineole	3.96	3.11	T				
104-87-0	4-Methylbenzaldehyde	5.13	3.11	T				
106-23-0	Citronellal	4.09	3.12	T				x
2385-77-5	(3R)-3,7-Dimethyloct-6-enal	4.09	3.12	T				
140-11-4	Benzyl acetate	4.13	3.13	T	Proposed; RT			
97-53-0	Eugenol	3.99	3.15	T				x
91-20-3	Naphthalene	3.62	3.17	T	CA, RT	U165		x
25586-57-6	Phenol, 2-methoxy(2-propenyl)-	3.75	3.18	T				x
106-30-9	Ethyl heptanoate	4.00	3.18	T			x	x
105-87-3	Geranyl acetate	4.18	3.18	T				x
6358-64-1	2,5-Dimethoxy-4-chloroaniline	4.20	3.20	T				x
492-88-6	Benzaldehyde, 3-ethoxy-2-hydroxy-	4.30	3.20	T				
93-89-0	Ethyl benzoate	4.21	3.21	T				x
106-27-4	Isopentyl butyrate	4.04	3.23	T			x	x
100-41-4	Ethylbenzene	4.24	3.23	T	CA		x	x
66-25-1	Hexanal	4.24	3.24	T				
100-42-5	Styrene	4.25	3.25	T	CA			x
6008-27-1	Nonalactone	3.63	3.26	T				x
104-55-2	3-Phenylprop-2-enal	4.10	3.26	T				x

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98-01-1	Furfural	4.31	3.27	T	Proposed; RT	U125		x
2050-01-3	Isopentyl isobutyrate	4.08	3.28	T				
14765-30-1	2-sec-Butylcyclohexan-1-one	4.15	3.28	T			x	x
118-61-6	Ethyl salicylate	4.30	3.30	T			x	x
120-50-3	Isobutyl benzoate	4.11	3.30	T				x
7440-36-0	Antimony & Antimony Compounds	4.31	3.31	Metals		Listed		x
121-39-1	Ethyl 2,3-epoxy-3-phenylpropionate	4.11	3.32	T				
99-87-6	p-Cymene	4.33	3.33	T				
7452-79-1	Ethyl 2-methylbutyrate	4.06	3.34	T			x	x
78-42-2	Tris(2-ethylhexyl) phosphate	4.34	3.34	PT			x	x
89-80-5	dl-Menthone	4.53	3.34	T				x
122-63-4	Benzyl propanoate	4.34	3.34	T				x
108-88-3	Toluene	4.65	3.35	T	RT, RDT	U220		x
104-61-0	gamma-Nonanolactone	4.17	3.35	T				x
104-67-6	5-Heptyldihydro-2(3H)-furanone	4.17	3.35	T				x
706-14-9	gamma-Decanolactone	4.19	3.35	T			x	x
1632-73-1	Fenchol	4.23	3.36	T				x
20921-04-4	Ethyl 3-(2-hydroxyphenyl)propanoate	4.23	3.36	T				
2217-02-9	(1R)-endo-(+)-Fenchyl alcohol	4.23	3.36	T				
134-20-3	Methyl 2-aminobenzoate	4.35	3.37	T				
120-47-8	Ethylparaben	4.23	3.39	T				
106-22-9	Citronellol	3.93	3.39	T				
80-26-2	alpha-Terpinyl acetate	4.39	3.39	T			x	x
93-15-2	Methyleugenol	4.40	3.40	T				x
99-93-4	4-Hydroxyacetophenone	4.32	3.41	T				
103-37-7	Benzyl butyrate	3.61	3.43	T				x
106-24-1	(2E)-3,7-Dimethyl-2,6-octadien-1-ol	4.30	3.44	T			x	x
334-48-5	Decanoic acid	3.88	3.45	T				
15932-80-6	Pulegone	4.40	3.45	T				x
6154-04-7	5-Amino-2-methyl-2H-tetrazole	4.41	3.45	P				x

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713-95-1	delta-Dodecalactone	4.45	3.45	T				
78-69-3	3,7-Dimethyl-3-octanol	4.22	3.46	T				x
100-52-7	Benzaldehyde	4.47	3.47	T				
99-49-0	dl-Carvone	4.47	3.47	T				x
89-78-1	dl-Menthol	4.75	3.47	T				x
624-54-4	Pentyl propionate	4.68	3.48	T				
138-86-3	Limonene	4.49	3.49	T				
131-17-9	Diallyl phthalate	3.66	3.49	T				
120-45-6	1-Phenylethyl propionate	3.66	3.49	T				x
93-28-7	Acetyeugenol	4.26	3.49	T				
65-85-0	Benzoic acid	4.96	3.50	Not PBT				x
122-00-9	p-Methylacetophenone	4.50	3.50	T				
7439-96-5	Manganese	4.50	3.50	Metals				
123-66-0	Ethyl hexanoate	4.01	3.53	T				
35408-14-1	8-Methylnona-3,7-dien-2-one	4.04	3.53	T				
109-21-7	Butyl butyrate	4.06	3.53	T				x
126-73-8	Tributyl phosphate	4.10	3.56	T				
89-81-6	Piperitone	4.08	3.57	T				
705-86-2	6-Pentyltetrahydro-2H-pyran-2-one	4.57	3.57	T				x
1330-20-7	Xylenes	4.59	3.59	T		U239		x
620-02-0	2-Furancarboxaldehyde, 5-methyl-	4.36	3.60	T				x
16543-55-8	N'-Nitrosornicotine	4.40	3.60	PT	CA	Listed		
115-95-7	Linalyl acetate	4.43	3.61	T				x
108-05-4	Vinyl acetate	4.61	3.61	T	CA, RT			x
103-36-6	Ethyl cinnamate	3.86	3.61	T				x
85-91-6	Methyl N-methylantranilate	4.30	3.61	T				x
77-83-8	Ethyl methylphenylglycidate	4.35	3.63	T				x
78-51-3	Tris(2-butoxyethyl) phosphate	4.50	3.64	T				x
93-51-6	2-Methoxy-4-methylphenol	5.18	3.64	T				x
1599-49-1	1,3-Dioxolane, 4-methyl-2-pentyl-	4.56	3.67	T				x
93-92-5	(+/-)-alpha-Methylbenzyl acetate	4.47	3.70	T				x

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127-63-9	Diphenylsulfone	3.99	3.72	PT				x
98-55-5	alpha-Terpineol	4.73	3.73	T				x
18278-34-7	4-Hydroxy-2-methoxybenzaldehyde	4.54	3.73	T				x
8000-41-7	Terpineol	4.75	3.75	T				x
7492-70-8	1-Butoxy-1-oxopropan-2-yl butanoate	3.86	3.75	T				x
76-22-2	Camphor	4.75	3.75	T				x
14073-97-3	(2S,5R)-2-Isopropyl-5-methylcyclohexan-1-one	4.76	3.76	T				x
1490-04-6	Menthol	4.36	3.77	T				x
6485-40-1	R-(-)-Carvone	4.78	3.78	T				x
99-76-3	Methylparaben	4.73	3.78	T			x	x
120-14-9	Veratraldehyde	4.88	3.79	T				
50-00-0	Formaldehyde	4.60	3.80	T	CA, RT	U122		x
110-82-7	Cyclohexane	4.80	3.80	T		U056		
13674-84-5	Tris(2-chloroisopropyl)phosphate	4.81	3.81	PT			x	x
101-97-3	Ethyl phenylacetate	4.01	3.81	T			x	x
609-40-5	Thiophene, 2-nitro-	4.57	3.81	PT			x	x
109-52-4	Pentanoic acid	4.82	3.82	Not PBT				
5579-78-2	epsilon-Decalactone	3.88	3.83	T				x
103-82-2	Phenylacetic acid	4.84	3.84	Not PBT			x	x
104-54-1	3-Phenyl-2-propen-1-ol	4.86	3.86	T				x
3681-71-8	(3Z)-3-Hexenyl acetate	4.55	3.86	T				x
67-56-1	Methanol	6.29	3.88	Not PBT		U154		x
57583-54-7	Tetraphenyl m-phenylene bis(phosphate)	4.89	3.89	PT				x
123-35-3	Myrcene	4.89	3.89	T				x
119-36-8	Methyl salicylate	4.90	3.90	T				x
10599-70-9	3-Acetyl-2,5-dimethylfuran	4.82	3.90	T				x
1124-11-4	Tetramethylpyrazine	5.04	3.90	T				x
628-63-7	Pentyl acetate	5.32	3.91	T				
106-70-7	Methyl hexanoate	4.79	3.91	T			x	x
121-33-5	4-Hydroxy-3-methoxybenzaldehyde	4.93	3.93	T				

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75-07-0	Acetaldehyde	4.95	3.95	Not PBT	CA, RT, AD	U001		
108-64-5	Ethyl isovalerate	4.51	3.97	T				x
624-41-9	2-Methylbutyl acetate	4.51	3.97	T				
5471-51-2	4-(4-Hydroxyphenyl)butan-2-one	4.91	3.97	T				x
79-09-4	Propionic acid	4.97	3.97	Not PBT	Proposed; RT			x
3658-77-3	4-Hydroxy-2,5-dimethyl-3(2H)furanone	4.60	3.97	T				x
84-66-2	Diethyl phthalate	4.51	3.99	T		U088		x
110-93-0	6-Methyl-5-hepten-2-one	4.99	3.99	T				
78-70-6	Linalool	4.67	3.99	T				
60-35-5	Acetamide	7.00	4.00	T	CA			
123-92-2	3-Methylbutyl acetate	5.00	4.00	T	Proposed; RT			x
71-43-2	Benzene	4.88	4.01	T	CA, CT, RDT	U019		x
123-86-4	Butyl acetate	5.01	4.01	T				x
105-53-3	Diethyl propanedioate	5.02	4.02	T				x
80-71-7	Cyclotene	5.04	4.04	T				
142-62-1	Hexanoic acid	5.05	4.05	Not PBT				x
131-11-3	Dimethyl phthalate	4.99	4.08	T		U102		x
101-41-7	Methyl phenylacetate	5.11	4.11	T				x
90-05-1	2-Methoxyphenol	5.12	4.12	T				x
123-11-5	4-Methoxybenzaldehyde	5.00	4.13	T				x
105-37-3	Ethyl propionate	5.14	4.14	T			x	x
91-10-1	2,6-Dimethoxyphenol	5.08	4.15	Not PBT				x
98-86-2	Acetophenone	5.18	4.18	Not PBT		U004		x
470-82-6	1,8-Cineol	4.97	4.19	T				
590-86-3	3-Methylbutanal	4.48	4.20	T				x
104-21-2	4-Methoxybenzyl acetate	4.70	4.20	T				
1193-11-9	2,2,4-Trimethyl-1,3-dioxolane	5.15	4.20	Not PBT				x
544-12-7	3-Hexen-1-ol	5.30	4.20	Not PBT			x	x

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100-51-6	Benzyl alcohol	5.09	4.21	Not PBT				x
109-60-4	Propyl acetate	5.21	4.21	T				x
115-96-8	Tris(2-chloroethyl) phosphate	5.21	4.21	PT			x	x
110-86-1	Pyridine	5.21	4.21	Not PBT		U196		x
92-48-8	6-Methyl coumarin	4.26	4.23	T				x
105-13-5	(4-Methoxyphenyl)methanol	5.25	4.25	Not PBT				
100-06-1	4'-Methoxyacetophenone	4.92	4.26	Not PBT				x
111-27-3	1-Hexanol	5.26	4.26	Not PBT				x
110-19-0	Isobutyl acetate	5.32	4.28	T	Proposed; RT			x
105-54-4	Ethyl butyrate	5.88	4.28	T				
79-31-2	2-Methylpropanoic acid	5.38	4.30	Not PBT				x
2568-25-4	1,3-Dioxolane, 4-methyl-2-phenyl-	5.26	4.30	P				x
121-32-4	3-Ethoxy-4-hydroxybenzaldehyde	5.13	4.31	T				x
68527-74-2	Phenol, 2-methoxy-4-(4-methyl-1,3-dioxolan-2-yl)-	5.04	4.32	Not PBT				x
6414-32-0	2-(4-Methoxyphenyl)-4-methyl-1,3-dioxolane	5.26	4.32	Not PBT				x
14667-55-1	2,3,5-Trimethylpyrazine	5.40	4.32	Not PBT				x
13925-03-6	2-Ethyl-6-methylpyrazine	5.45	4.36	Not PBT				x
77-93-0	Triethyl citrate	5.51	4.37	Not PBT				x
81-07-2	Saccharin	5.37	4.37	PT				x
87-28-5	2-Hydroxyethyl salicylate	4.82	4.38	T				x
4940-11-8	2-Ethyl-3-hydroxy-4-pyrone	5.38	4.38	T				x
64091-91-4	4-(N-Methyl-N-nitrosamino)-1-(3-pyridyl)-1-butanone (NNK)	5.52	4.38	P	CA			
64-19-7	Acetic acid	5.39	4.39	Not PBT	Proposed; RT			x
106-65-0	Dimethyl succinate	5.45	4.40	Not PBT			x	x
881-68-5	Benzaldehyde, 4-(acetyloxy)-3-methoxy-	4.94	4.41	T				x
556-52-5	Glycidol	5.44	4.44	T	Proposed; CA			x
107-92-6	Butanoic acid	5.44	4.44	Not PBT				x

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928-96-1	(Z)-3-Hexen-1-ol	5.50	4.50	Not PBT			x	x
1320-51-0	(Hydroxyethyl)urea	5.09	4.54	Not PBT			x	x
98-00-0	Furfuryl alcohol	5.56	4.56	Not PBT			x	x
104-50-7	4-Hydroxyoctanoic acid lactone	4.34	4.58	T			x	x
698-76-0	delta-Octanolactone	4.34	4.58	T				
513-86-0	Acetoin	5.45	4.58	Not PBT	Proposed; RT			x
96-48-0	4-Butyrolactone	5.59	4.59	Not PBT				
6290-17-1	Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate	4.72	4.59	T				
141-97-9	Ethyl acetoacetate	5.60	4.60	Not PBT	Proposed; RT			x
105-57-7	Acetal	5.67	4.61	Not PBT				x
462-95-3	Diethoxymethane	5.65	4.65	Not PBT				x
102-76-1	Triacetin	5.66	4.66	Not PBT				x
118-71-8	Maltol	5.64	4.66	T				
123-51-3	Isopentyl alcohol	5.70	4.68	Not PBT			x	
67-64-1	Acetone	6.60	4.69	Not PBT	RT	U002		x
547-63-7	Propanoic acid, 2-methyl-, methyl ester	4.94	4.70	T				
108-50-9	2,6-Dimethylpyrazine	5.76	4.72	Not PBT				
123-32-0	2,5-Dimethylpyrazine	5.76	4.72	Not PBT				x
5910-89-4	Pyrazine, 2,3-dimethyl-	5.76	4.72	Not PBT				x
64-17-5	Ethanol	6.36	4.75	Not PBT				x
116-09-6	Hydroxyacetone	5.48	4.77	Not PBT				x
137-00-8	Thiamine thiozole	5.76	4.77	Not PBT				x
141-78-6	Ethyl acetate	5.80	4.80	T	Proposed; RT	U112		x
60-12-8	2-Phenylethanol	5.63	4.82	Not PBT				
123-25-1	Diethyl butanedioate	5.15	4.84	T				x
79-20-9	Methyl acetate	5.67	4.85	T	Proposed; RT			x
59276-33-4	4-(Dimethoxymethyl)-1,2-dimethoxybenzene	5.96	4.96	Not PBT				
71-41-0	1-Pentanol	5.65	5.01	Not PBT				

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6920-22-5	1,2-Hexanediol	4.75	5.04	Not PBT				x
78-83-1	2-Methyl-1-propanol	6.04	5.04	Not PBT		U140		x
119-84-6	3,4-Dihydrocoumarin	5.28	5.11	T				x
109-08-0	2-Methylpyrazine	5.56	5.11	Not PBT				x
112-34-5	2-(2-Butoxyethoxy)ethanol	6.25	5.20	Not PBT				
1119-40-0	Dimethyl glutarate	4.76	5.23	T				
1122-62-9	2-Acetylpyridine	5.65	5.23	Not PBT				x
6214-01-3	1,2-Propanediol, 2-acetate	6.00	5.26	Not PBT				x
695-06-7	gamma-Caprolactone	4.80	5.32	Not PBT				
116-53-0	2-Methylbutanoic acid	4.81	5.32	Not PBT				x
112-36-7	Diethylene glycol diethyl ether	6.43	5.43	Not PBT				
16777-87-0	3,3-Diethoxy-1-propanol	6.58	5.52	Not PBT				x
74685-84-0		5.49	5.54	BT				x
1708-40-3	1,3-Dioxan-5-ol, 2-phenyl-	6.56	5.56	Not PBT				
108-29-2	4-Pentanolide	5.00	5.68	Not PBT				x
78-40-0	Triethyl phosphate	5.58	5.68	T				x
107-21-1	Ethylene glycol	7.18	5.93	Not PBT	Proposed; RT, RDT			
56-81-5	Glycerol	6.94	5.94	Not PBT	Proposed; RT			
22047-25-2	Acetylpyrazine	6.88	5.94	Not PBT				x
496-76-4	2,6-Dihydroxypyrimidin-5(4H)-one	7.08	5.97	Not PBT				x
143-24-8	2,5,8,11,14-Pentaoxapentadecane	7.00	6.00	Not PBT				
97-64-3	Ethyl lactate	5.81	6.00	Not PBT				x
67-63-0	Isopropanol	6.65	6.01	Not PBT				
765-70-8	3-Methyl-1,2-cyclopentanedione	6.96	6.04	Not PBT				x
4254-15-3	(+)-1,2-Propanediol	6.75	6.08	Not PBT			x	
1874-62-0	3-Ethoxypropane-1,2-diol	7.08	6.18	BT				
112-49-2	Triethylene glycol dimethyl ether	7.20	6.20	Not PBT				x
557-25-5	Butanoic acid, 2,3-dihydroxypropyl ester	6.00	6.20	Not PBT				
110-98-5	1,1'-Oxybis-2-propanol	6.50	6.20	Not PBT				

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106-62-7	1-propanol, 2-(2-hydroxypropoxy)-	7.11	6.20	Not PBT				
600-14-6	2,3-Pentanedione	7.15	6.23	Not PBT	Proposed; RT			
542-59-6	1,2-Ethandiol, 1-acetate	5.33	6.30	Not PBT				
57-55-6	1,2-Propylene glycol	6.63	6.41	Not PBT	Proposed; RT			
3610-27-3	Ethanol, 2-[2-(2-methoxyethoxy)ethoxy]-, 1-acetate	6.20	6.46	Not PBT				
25395-31-7	Diacetain glycerol	5.68	6.56	Not PBT				
431-03-8	2,3-Butanedione	7.45	6.58	Not PBT	Proposed; RT			
3885-29-8	Methyl 5-oxotetrahydrofuran-2-carboxylate	6.30	6.64	Not PBT				×
106-61-6	Acetin, 1-mono-	6.48	6.95	Not PBT				×
26446-35-5	Acetin	6.48	6.95	Not PBT				
50-70-4	D-Glucitol	9.04	8.30	Not PBT				×
5617-32-3	Heptaethylene glycol	9.72	8.41	Not PBT			×	×
57-50-1	Sucrose	11.04	9.61	Not PBT				

References

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