

## Full Tier 1 Chemical List for CLAP.

Code	IUPAC name	Trivial name	CAS #	Empirical Formula	DBE	MW (g/mol)	BP (°C, @760 mmHg)	pKa	logP	Refractive Index
RM1	[3-[3-(3,5-ditert-butyl-4-hydroxyphenyl)propanoyloxy]-2,2-bis[3-(3,5-ditert-butyl-4-hydroxyphenyl)propanoyloxymethyl]propyl] 3-(3,5-ditert-butyl-4-hydroxyphenyl)propanoate	Irganox 1010	6683-19-8	C73H108O12	20	1177.6	779.0	11.71	23.00	N/A
RM2	octadecyl 3-(3,5-ditert-butyl-4-hydroxyphenyl)propanoate	Irganox 1076	2082-79-3	C35H62O3	5	530.9	568.0	12.33	13.93	N/A
RM3	tris(2,4-ditert-butylphenyl) phosphite	Irgafos 168	31570-04-4	C42H63O3P	11.5	646.9	361.0	N/A	17.56	N/A
RM4	2,6-ditert-butyl-4-methylphenol	Butylated hydroxytoluene	128-37-0	C15H24O	4	220.4	265.0	12.75	5.30	1.499
RM5	2,4-ditert-butylphenol	2,4-Di-tert-butyl phenol	96-76-4	C14H22O	3	206.3	264.0	11.56	5.19	1.499
RM6	2,4-dimethylphenol	2,4-Dimethylphenol	105-67-9	C8H10O	3	122.2	212.0	10.60	2.30	1.540
RM7	2-tert-butyl-4-methoxyphenol	3-tert-Butyl-4-hydroxyanisole	25013-16-5	C11H16O2	4	180.3	268.0	10.58	3.50	1.491
RM8	bis(2-ethylhexyl) benzene-1,2-dicarboxylate	Di-(2-ethylhexyl)phthalate	117-81-7	C24H38O4	6	390.6	386.0	-6.70	7.60	1.486
RM9	dibutyl benzene-1,2-dicarboxylate	Dibutylphthalate	84-74-2	C16H22O4	6	278.3	340.0	-6.70	4.50	1.499
RM10	diphenyl benzene-1,2-dicarboxylate	Diphenyl phthalate	84-62-8	C20H14O4	14	318.3	497.0	N/A	4.10	1.616

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RM11	2- <i>O</i> -benzyl 1- <i>O</i> -butyl benzene-1,2-dicarboxylate	Benzyl butyl phthalate	85-68-7	C19H20O4	10	312.4	370.0	-6.70	4.73	1.553
RM12	tris(2-ethylhexyl) benzene-1,2,4-tricarboxylate	Tris (2-ethylhexyl) trimellitate	3319-31-1	C33H54O6	7	546.8	414.0	N/A	12.80	1.488
RM13	azepan-2-one	Caprolactam	105-60-2	C6H11NO	1.5	113.2	271.0	14.99	-0.32	1.446
RM14	4-[2-(4-hydroxyphenyl)propan-2-yl]phenol	Bisphenol A	80-05-7	C15H16O2	8	228.3	360.0	10.29	3.43	1.599
RM15	( <i>Z</i> )-docos-13-enamide	Erucamide	112-84-5	C22H43NO	1.5	337.6	474.0	16.61	8.87	1.469
RM16	( <i>Z</i> )-octadec-9-enamide	Oleamide	301-02-0	C18H35NO	1.5	281.5	200.0	16.92	7.07	1.470
RM17	butyl octadecanoate	Butyl stearate	123-95-5	C22H44O2	1	340.6	343.0	-7.00	10.27	1.448
RM18	2-(benzotriazol-2-yl)-4,6-ditert-butylphenol	Tinuvin 320	3846-71-7	C20H25N3O	10	323.4	444.0	9.41	7.22	1.586
RM19	2,2,4,4,6,6,8,8-octamethyl-1,3,5,7,2,4,6,8-tetraoxatetrasiloxane	D4 siloxane	556-67-2	C8H24O4Si4	1	296.6	176.0	N/A	6.70	1.423
RM20	2,2,4,4,6,6,8,8,10,10,12,12-dodecamethyl-1,3,5,7,9,11-hexaoxa-2,4,6,8,10,12-hexasilacyclododecane	D6 Siloxane	540-97-6	C12H36O6Si6	1	444.9	210.0	N/A	8.87	1.431
RM21	bis(2-methylpropyl) hexanedioate	Diisobutyl adipate	141-04-8	C14H26O4	2	258.4	293.0	-6.70	3.85	1.439
RM22	bis(6-methylheptyl) nonanedioate	Diisooctyl azelate	26544-17-2	C25H48O4	2	412.7	NA	N/A	9.33	1.453
RM23	dibutyl decanedioate	Dibutyl sebacate	109-43-3	C18H34O4	2	314.5	179.0	-6.70	5.97	1.448
RM24	1- <i>O</i> -heptyl 6- <i>O</i> -nonyl hexanedioate	Heptylnonyl Adipate	68515-75-3	C22H42O4	2	370.6	224.0	N/A	8.47	1.452
RM25	<i>N</i> -benzyl-1-phenylmethanamine	Dibenzylamine	103-49-1	C14H15N	8	197.3	300.0	18.25	3.42	1.581
RM26	benzoic acid	Benzoic acid	65-85-0	C7H6O2	5	122.1	249.0	4.00	1.89	1.564

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RM27	2-ethylhexanoic acid	2-Ethylhexanoic acid	149-57-5	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	1	144.2	228.0	4.82	2.72	1.435
RM28	1-chloro-4-(4-chlorophenyl)sulfonylbenzene	Bis(4-chlorophenyl) sulfone	80-07-9	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>2</sub> S	8	287.2	397.0	N/A	3.90	1.610
RM29	2,6-ditert-butyl-4-(hydroxymethyl)phenol	3,5-Di-tert-butyl-4-hydroxybenzyl alcohol	88-26-6	C <sub>15</sub> H <sub>24</sub> O <sub>2</sub>	4	236.4	214.0	12.01	3.67	1.519
RM30	1,3-ditert-butylbenzene	1,3-Di-tert-butylbenzene	1014-60-4	C <sub>14</sub> H <sub>22</sub>	4	190.3	223.6	N/A	5.59	1.478
RM31	tris(2,4-ditert-butylphenyl) phosphate	Tris(2,4-ditert-butylphenyl) phosphate	95906-11-9	C <sub>42</sub> H <sub>63</sub> O <sub>4</sub> P	12	662.9	609.8	N/A	13.12	1.514
RM32	hexadecanoic acid	Palmitic acid	57-10-3	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	1	256.4	352.0	4.95	7.17	1.454
RM33	N-(1,3-benzothiazol-2-ylsulfanyl)-2-methylpropan-2-amine	TBBS	95-31-8	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> S <sub>2</sub>	7.5	238.4	344.0	1.25	4.49	1.642
RM34	1,2-bis(2-methylphenyl)guanidine	Ditolylguanidine	97-39-2	C <sub>15</sub> H <sub>17</sub> N <sub>3</sub>	9	239.3	396.0	10.32	3.77	1.585
RM35	1-N-phenyl-4-N-propan-2-ylbenzene-1,4-diamine	IPPD	101-72-4	C <sub>15</sub> H <sub>18</sub> N <sub>2</sub>	8	226.3	378.0	6.76	2.83	1.634
RM36	1,3,5-tris[(3,5-ditert-butyl-4-hydroxyphenyl)methyl]-1,3,5-triazinane-2,4,6-trione	Irganox 3114	27676-62-6	C <sub>48</sub> H <sub>69</sub> N <sub>3</sub> O <sub>6</sub>	16	784.1	NA	11.45	10.34	1.567
RM37	5-chloro-2-(2,4-dichlorophenoxy)phenol	Triclosan	3380-34-5	C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub> O <sub>2</sub>	8	289.5	290.0	7.90	5.17	1.632

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RM38	zinc;1-oxidopyridin-1-ium-2-thiolate	Zinc pyrithione	13463-41-7	C10H8N2O2S2Zn	8	317.7	NA	N/A	0.90	N/A
RM39	dimethyl-octadecyl-(3-trihydroxysilylpropyl)azanium;chloride	AEM 5772	199111-50-7	C23H52ClNO3Si	-2	454.2	NA	N/A	N/A	N/A
RM40	2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydrochromen-6-ol	Vitamin E	10191-41-0	C29H50O2	5	430.7	485.9	11.40	11.90	1.495
RM41	2- <i>tert</i> -butyl-6-[[3- <i>tert</i> -butyl-5-ethyl-2-hydroxyphenyl)methyl]-4-ethylphenol	Cyanox 425	88-24-4	C25H36O2	8	368.6	452.0	11.37	8.09	1.544
RM42	4-(1-phenylethyl)- <i>N</i> -[4-(1-phenylethyl)phenyl]aniline	DUSANTOX 80	60160-25-0	C28H27N	16	377.5	288.0	N/A	7.64	1.626
RM43	(piperidine-1-carbothioyltrisulfanyl)piperidine-1-carbodithioate	Tetrone A	120-54-7	C12H20N2S6	4	384.7	510.0	0.85	5.50	1.730
RM44	2-[2-[3-(3,5- <i>ditert</i> -butyl-4-hydroxyphenyl)propanoyloxy]ethylsulfanyl]ethyl 3-(3,5- <i>ditert</i> -butyl-4-hydroxyphenyl)propanoate	Irganox 1035	41484-35-9	C38H58O6S	10	642.9	659.0	12.02	10.64	1.533
RM45	3,9-bis[2,4-bis(2-phenylpropan-2-yl)phenoxy]-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane	ANTIOXIDAN T 852	154862-43-8	C53H58O6P2	25	853.0	778.0	N/A	15.75	N/A
RM46	2-[3,5-bis[2-[3-(3,5- <i>ditert</i> -butyl-4-hydroxyphenyl)propanoyloxy]ethyl]-2,4,6-trioxo-1,3,5-triazinan-1-yl]ethyl 3-(3,5- <i>ditert</i> -butyl-4-hydroxyphenyl)propanoate	Irganox 3125	34137-09-2	C60H87N3O12	19	1042.4	922.0	11.85	12.06	1.543
RM47	<i>N,N</i> -bis(2-hydroxyethyl)dodecanamide	Lauramide DEA	120-40-1	C16H33NO3	1	287.4	443.0	14.16	3.94	1.480
RM48	2,3-dihydroxypropyl octadecanoate	Monostearin	123-94-4	C21H42O4	1	358.6	476.9	13.39	7.23	1.469
RM49	1,3-benzothiazole	Benzothiazole	95-16-9	C7H5NS	6	135.2	227.0	0.85	2.01	1.689

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RM50	<i>N,N</i> -dimethyl-1-phenylmethanamine	BDMA	103-83-3	C9H13N	4	135.2	181.0	9.62	1.98	1.517
RM51	4- <i>tert</i> -butylphenol	4- <i>tert</i> -Butylphenol	98-54-4	C10H14O	4	150.2	234.0	9.67	3.17	1.514
RM52	4-(2-methylbutan-2-yl)phenol	4- <i>tert</i> -Amylphenol	80-46-6	C11H16O	4	164.2	262.5	9.64	3.70	1.510
RM53	4-[[4-aminophenyl)methyl]aniline	4,4'-Methylenedi aniline	101-77-9	C13H14N2	8	198.3	398.0	5.32	1.64	1.660
RM54	6-(dibutylamino)-1 <i>H</i> -1,3,5-triazine-2,4-dithione	6-(Dibutylamino)-1,3,5-triazine-2,4-dithiol	29529-99-5	C11H20N4S2	4	272.4	343.7	6.06	2.12	1.622
RM55	<i>N</i> -(1,3-benzothiazol-2-ylsulfanyl)cyclohexanamine	CBS	95-33-0	C13H16N2S2	7	264.4	410.4	0.59	5.32	1.665
RM56	3 <i>H</i> -1,3-benzothiazole-2-thione	2-Mercaptobenzothiazole	149-30-4	C7H5NS2	6	167.3	281.3	9.80	2.41	1.757
RM57	octadecanoic acid	Stearic Acid	57-11-4	C18H36O2	1	284.5	359.4	4.70	8.22	1.456
RM58	1,4-diphenylbenzene	<i>p</i> -Terphenyl	92-94-4	C18H14	12	230.3	400.0	4.75	5.63	1.602
RM59	<i>N</i> -[2-(octadecanoylamino)ethyl]octadecanamide	Ethylene distearamide	110-30-5	C38H76N2O2	2	593.0	720.3	15.53	14.99	1.467
RM60	3,4-dimethylbenzaldehyde	3,4-Dimethylbenzaldehyde	5973-71-7	C9H10O	5	134.2	225.3	N/A	2.56	1.551
RM61	2,2-dimethyl- <i>N</i> -phenylpropanamide	Pivalanilide	6625-74-7	C11H15NO	5	177.2	323.5	15.12	2.31	1.545
RM62	sodium;1,3,7,9-tetratert-butyl-11-oxido-5 <i>H</i> -	Sodium bis(2,2-methylene-	85209-91-2	C29H42NaO4P	9.5	508.6	510.4	2.10	0.80	N/A

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	benzo[d][1,3,2]benzodioxaphosphocine 11-oxide	bis(4,6-di-tert-butylphenyl) phosphate)								
<b>RM63</b>	triethyl phosphate	Triethyl phosphate	78-40-0	C6H15O4P	0	182.2	216.0	-9.10	1.08	1.406
<b>RM64</b>	2,3-diacetyloxypropyl acetate	Triacetin	102-76-1	C9H14O6	3	218.2	258.0	-6.50	-0.24	1.435
<b>RM65</b>	triethyl 2-hydroxypropane-1,2,3-tricarboxylate	Triethyl citrate	77-93-0	C12H20O7	3	276.3	294.0	10.28	1.49	1.462
<b>RM66</b>	[2,2,4-trimethyl-3-(2-methylpropanoyloxy)pentyl] 2-methylpropanoate	TXIB	6846-50-0	C16H30O4	2	286.4	280.0	N/A	4.04	1.441
<b>RM67</b>	methyl (Z)-octadec-9-enoate	Methyl oleate	112-62-9	C19H36O2	2	296.5	351.4	N/A	8.16	1.454
<b>RM68</b>	propan-2-yl hexadecanoate	Isopropyl palmitate	142-91-6	C19H38O2	1	298.5	340.7	N/A	8.49	1.443
<b>RM69</b>	diphenyl benzene-1,4-dicarboxylate	Diphenyl terephthalate	1539-04-4	C20H14O4	14	318.3	496.6	N/A	5.39	1.616
<b>RM70</b>	6-amino-4-(ethylamino)-1 <i>H</i> -1,3,5-triazin-2-one	DEHS	7313-54-4	C5H9N5O	4	155.2	464.4	7.53	1.13	1.700
<b>RM71</b>	tributyl 2-hydroxypropane-1,2,3-tricarboxylate	Tributyl citrate	77-94-1	C18H32O7	3	360.5	389.8	11.30	4.68	1.465
<b>RM72</b>	bis(6-methylheptyl) benzene-1,2-dicarboxylate	Diisooctyl phthalate	27554-26-3	C24H38O4	6	390.6	384.9	N/A	8.71	1.489
<b>RM73</b>	bis(2-ethylhexyl) benzene-1,4-dicarboxylate	DOTP	6422-86-2	C24H38O4	11	390.6	400.0	N/A	9.55	1.489
<b>RM74</b>	tributyl 2-acetyloxypropane-1,2,3-tricarboxylate	Acetyltributyl citrate	77-90-7	C20H34O8	4	402.5	418.1	N/A	6.92	1.458

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RM75	dioctyl nonanedioate	Dioctyl azelate	2064-80-4	C25H48O4	2	412.7	431.3	N/A	9.69	1.454
RM76	bis(2-ethylhexyl) decanedioate	Bis(2-ethylhexyl)s ebacate	122-62-3	C26H50O4	2	426.7	435.5	N/A	9.86	1.454
RM77	bis(7-methyloctyl) benzene-1,2-dicarboxylate	Diisononyl phthalate	28553-12-0	C26H42O4	6	418.6	435.5	N/A	10.14	1.489
RM78	bis(7-methyloctyl) cyclohexane-1,2-dicarboxylate	Diisononyl hexahydrophthalate	166412-78-8	C26H48O4	3	424.7	489.6	N/A	9.69	1.466
RM79	bis(8-methylnonyl) hexanedioate	Diisodecyl adipate	27178-16-1	C26H50O4	2	426.7	428.0	N/A	10.23	1.454
RM80	dicyclohexyl benzene-1,2-dicarboxylate	Dicyclohexyl phthalate	84-61-7	C20H26O4	8	330.4	425.8	N/A	5.76	1.544
RM81	trihexyl 2-butanoyloxypropane-1,2,3-tricarboxylate	Butyryl trihexyl citrate	82469-79-2	C28H50O8	4	514.7	522.3	N/A	11.17	1.462
RM82	tris(6-methylheptyl) benzene-1,2,4-tricarboxylate	Triisooctyl trimellitate	27251-75-8	C33H54O6	7	546.8	585.0	N/A	12.80	1.488
RM83	bis(2-ethylhexyl) cyclohexane-1,2-dicarboxylate	di(2-ethylhexyl) hexahydrophthalate	84-71-9	C24H44O4	3	396.6	463.9	N/A	8.63	1.465
RM84	Tri(n-octyl, n-decyl) trimellitate	Tri(n-octyl, n-decyl) trimellitate	67989-23-5*	C72H120O12	13	1177.7	583.0	N/A	20.82	N/A
RM85	2-benzofuran-1,3-dione	Phthalic anhydride	85-44-9	C8H4O3	7	148.1	295.0	2.97	1.60	1.613
RM86	2H-benzotriazole	Benzotriazole	95-14-7	C6H5N3	6	119.1	359.2	1.60	1.34	1.715

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RM87	2-(1,3-benzothiazol-2-yl)phenol	2-(benzo[d]thiazol-2-yl)phenol	3411-95-8	C13H9NOS	10	227.3	402.2	8.21	4.53	1.719
RM88	2-tert-butyl-6-(5-chlorobenzotriazol-2-yl)-4-methylphenol	Tinuvin 326	3896-11-5	C17H18ClN3O	10	315.8	460.4	9.31±0.48	6.58	1.628
RM89	(2-hydroxy-4-octoxyphenyl)-phenylmethanone	Octabenzone	1843-05-6	C21H26O3	9	326.4	457.9	7.59	7.36	1.548
RM90	2-(benzotriazol-2-yl)-4,6-bis(2-methylbutan-2-yl)phenol	Tinuvin 328	25973-55-1	C22H29N3O	10	351.5	469.1	8.85	8.28	1.575
RM91	bis(2,2,6,6-tetramethylpiperidin-4-yl)decanedioate	Tinuvin 770	52829-07-9	C28H52N2O4	4	480.7	499.8	10.49	7.32	1.498
RM92	(2,4-dihydroxyphenyl)-phenylmethanone	Benzophenone-1	131-56-6	C13H10O3	9	214.2	409.0	7.72	3.17	1.648
RM93	2-(benzotriazol-2-yl)-4-methylphenol	Tinuvin P	2440-22-4	C13H11N3O	10	225.3	423.8	8.15	4.30	1.682
RM94	2-(benzotriazol-2-yl)-4-(2,4,4-trimethylpentan-2-yl)phenol	Octrizole	3147-75-9	C20H25N3O	10	323.4	471.8	8.07	7.29	1.585
RM95	2-(benzotriazol-2-yl)-4,6-bis(2-phenylpropan-2-yl)phenol	Tinuvin 234	70321-86-7	C30H29N3O	18	447.6	589.3	9.00	9.21	1.619
RM96	imidazolidine-2-thione	Ethylene thiourea	96-45-7	C3H6N2S	2	102.1	148.3	15.01	-0.66	1.626
RM97	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-nonadecafluorodecanoic acid	PFDA	335-76-2	C10HF19O2	1	514.1	219.0	0.52	9.53	1.289
RM98	2-ethylhexan-1-ol	2-Ethylhexanol	104-76-7	C8H18O	0	130.2	184.0	15.06	2.82	1.426
RM99	azacyclotridecan-2-one	Lauro lactam	947-04-6	C12H23NO	2	197.3	314.9	16.91	3.06	1.440
RM100	tetradecane	Tetradecane	629-59-4	C14H30	0	198.4	253.9	N/A	8.19	1.429
RM101	2-hydroxy-2-methyl-1-phenylpropan-1-one	benzoyl isopropanol	7473-98-5	C10H12O2	5	164.2	260.8	13.23	1.13	1.533



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RM102	2-phenylpropan-2-ol	2-Phenyl-2-propanol	617-94-7	C9H12O	4	136.2	202.0	14.49	1.73	1.518	
RM103	dodec-1-ene	1-Dodecene	112-41-4	C12H24	1	168.3	213.9	N/A	6.62	1.431	
RM104	2-dodecylbenzenesulfonic acid	Dodecylbenzene sulfonic acid	27176-87-0	C18H30O3S	4	326.5	204.5	0.70	6.78	1.510	
RM105	dodecyl 3-(3-dodecoxy-3-oxopropyl)sulfanylpropanoate	Dilauryl thiodipropionate	123-28-4	C30H58O4S	2	514.8	580.8	N/A	12.88	1.472	
RM106	2-(2-ethoxyethoxy)ethanol	Ethyl carbitol	111-90-0	C6H14O3	0	134.2	202.0	14.37	-0.62	1.420	
Ranges of physicochemical values of listed chemicals					Min	-2.0	102.1	148.3	-9.1	-0.7	1.289
					Max	25	1177.7	922	18.25	23	1.757

\* In this test, commercially available RM84 is comprised of a blend of tri-n-octyl trimellitate (CAS# 89-04-3, MW 546.8) and tri-n-decyl trimellitate (CAS# 4130-35-2, MW 630.9). However, the combined molecular weight is depicted in this table according to the manufacturer's information.