

GC Chemical Master List and Associated Physicochemical Properties

Code	Trivial name/ acronym	CAS #	Empirical Formula	Double Bond Equivalents (DBE)	Mol. Wt (g/mol)	Boiling Point (°C)	pKa	logP
A1	Irganox 1010; Naugard 10	6683-19-8	C73H108O12	20	1177.6	779	11.71± 0.40	19.4
A2	Irganox 1076	2082-79-3	C35H62O3	5	530.9	568	12.3	13.8
A3	Irgafos 168; Alakanox 240; Naugard 524; Ultrinox 668	31570-04-4	C42H63O3P	11.5	646.9	361	N/A	15.5
A4	Butylated hydroxytoluene (BHT)	128-37-0	C15H24O	4	220.4	265	12.8	5.3
A5	2,4-Di-t-butyl phenol	96-76-4	C14H22O	3	206.3	264	11.6	4.9
A6	2,4-Dimethylphenol	105-67-9	C8H10O	4	122.2	212	10.6	2.6
A7	2,4-Dimethylphenol-3,5,6-d3	93951-75-8	C8D3H7O	4	125.2	212	10.6	
A8	2(3)-Tert-butyl-4-methoxy phenol (BHA)	25013-16-5	C11H16O2	4	180.3	268	10.6	3.5
A9	Di-(2-ethylhexyl) phthalate (DEHP)	117-81-7	C24H38O4	6	390.6	386	-6.70	7.4
A10	Dibutylphthalate (DBP)	84-74-2	C16H22O4	6	278.3	340	-6.70	4.7
A11	Diphenyl phthalate (DPP)	84-62-8	C20H14O4	14	318.3	400-405		4.1
A12	Benzyl butyl phthalate	85-68-7	C19H20O4	10	312.4	370	-6.70	4.9
A13	Tris (2-ethylhexyl) trimellitate	3319-31-1	C33H54O6	7	546.8	414		10.4
A14	Caprolactam	105-60-2	C6H11NO	1.5	113.2	271	14.99	-0.1
A15	Bisphenol A	80-05-7	C15H16O2	8	228.3	360	10.3	3.3
A16	Erucamide	112-84-5	C22H43NO	1.5	337.6	474	16.6	8.8
A17	Oleamide	301-02-0	C18H35NO	1.5	281.5	200	16.92	6.6
A18	Butyl stearate	123-95-5	C22H44O2	1	340.6	343	-7.0	9.8
A19	Tinuvin 320	3846-71-7	C20H25N3O	10	323.4	444	9.41	5.6
A20	D4 siloxane	556-67-2	C8H24O4Si4	1	296.6	176		6.7
A21	D6 Siloxane	540-97-6	C12H36O6Si6	1	444.9	210		9.1
A22	Diisobutyl adipate	141-04-8	C14H26O4	2	258.4	293	-6.7	3.2
A23	Diisooctyl azelate	26544-17-2	C25H48O4	2	412.7	NA		8.5
A24	Dibutyl sebacate	109-43-3	C18H34O4	2	314.5	179	-6.7	5.3
A25	Di(n-heptyl, n-nonyl) adipate	68515-75-3	C22H42O4	2	370.6	224		7.55
A26	Dibenzylamine	103-49-1	C14H15N	8	197.3	300	18.25	2.7

GC Chemical Master List and Associated Physicochemical Properties

Code	Trivial name/ acronym	CAS #	Empirical Formula	Double Bond Equivalents (DBE)	Mol. Wt (g/mol)	Boiling Point (°C)	pKa	logP
A27	Benzoic acid	65-85-0	C7H6O2	5	122.1	249	4	1.9
A28	2-Ethylhexanoic acid	149-57-5	C8H16O2	1	144.2	226 - 229	4.819	2.6
A29	Bis(4-chlorophenyl) sulfone	80-07-9	C12H8Cl2O2S	8	287.2	397		3.9
A30	3,5-Di- <i>tert</i> -butyl-4-hydroxybenzyl alcohol	88-26-6	C15H24O2	4	236.4	214	12.01	4
A31	1,3-Di- <i>tert</i> -butylbenzene	1014-60-4	C14H22	4	190.3	106-107		5.8
A32	Tris(2,4-di- <i>tert</i> -butylphenyl)phosphate	95906-11-9	C42H63O4P	12	662.9	609.8± 55	N/A	13.12
A33	Palmitic acid	57-10-3	C16H32O2	1	256.4	352	4.95	7.17
B1	TBBS; BBTs; NTBTS	95-31-8	C11H14N2S2	7.5	238.4	344	1.25±0.70	4.49
B2	1,3-Di- <i>o</i> -tolylguanidine	97-39-2	C15H17N3	9	239.3	396	10.32±0.10	3.77
B3	Santoflex® IPPD	101-72-4	C15H18N2	8	226.3	378	6.76±0.32	2.83
B4	Irganox 3114	27676-62-6	C48H69N3O6	16	784.1	NA	11.45±0.40	12.8
B5	Triclosan, Irgasan	3380-34-5	C12H7Cl3O2	8	289.5	290	7.9	5.17
B6	Zinc pyrithione	13463-41-7	C10H8N2O2S2Zn	8	317.7	NA	NA	0.9
B7	gelest HE4001 & 4005	199111-50-7	C23H52ClNO3Si	-2	454.2	NA	NA	NA
B8	Irganox® E 201	10191-41-0	C29H50O2	5	430.7	450	11.40±0.40	11.9
B9	Cyanox® 425	88-24-4	C25H36O2	8	368.6	452	11.37±0.48	8.09
B10	Naugard® 635	60160-25-0	C28H27N	16	377.5	288	NA	8
B11	Dipentamethylenethiuram tetrasulfide	120-54-7	C12H20N2S6	4	384.7	510	0.85±0.20	5.5
B12	Irganox® 1035	41484-35-9	C38H58O6S	10	642.9	659	12.02±0.40	8.6728
B13	3,9-bis(2,4-Dicumylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5,5] undecane	154862-43-8	C53H58O6P2	25	853.0	NA	NA	14.4
B14	Irganox® 3125	34137-09-2	C60H87N3O12	19	1042.4	NA	11.85	13.7
B15	lauric acid diethanolamide	120-40-1	C16H33NO3	1	287.4	443	14.161	2.7205
B16	Glyceryl monostearate	123-94-4	C21H42O4	1	358.6	477	13.385	7.23
B17	Benzothiazole	95-16-9	C7H5NS	6	135.2	227	0.85	2.01
B18	N,N-Dimethylbenzylamine	103-83-3	C9H13N	4	135.2	181	9.615	1.98
B19	4- <i>tert</i> -Butylphenol	98-54-4	C10H14O	4	150.2	234	9.667	3.17

GC Chemical Master List and Associated Physicochemical Properties

Code	Trivial name/ acronym	CAS #	Empirical Formula	Double Bond Equivalents (DBE)	Mol. Wt (g/mol)	Boiling Point (°C)	pKa	logP
B20	4-tert-Amylphenol	80-46-6	C11H16O	4	164.2	248	9.644	3.7
B21	4,4'-Methylenedianiline	101-77-9	C13H14N2	8	198.3	398	5.32	1.64
B22	6-(Dibutylamino)-1,3,5-triazine-2,4-dithiol	29529-99-5	C11H20N4S2	4	272.4	NA	6.06	2.8
B23	N-Cyclohexyl-2-benzothiazolylsulfenamide	95-33-0	C13H16N2S2	7	264.4	410	0.59	5.32
B24	Perkacit® MBT	149-30-4	C7H5S2N	6	167.3	305	9.8	2.38
B25	Stearic Acid	57-11-4	C18H36O2	1	284.5	383	4.702	6.3325
B26	p-Terphenyl	92-94-4	C18H14	12	230.3	389	4.75	5.63
B27	N,N-ethylene bis(Stearamide)	110-30-5	C38H76N2O2	2	593.0	720	15.53	14.99
B28	3,4-Dimethylbenzaldehyde	5973-71-7	C9H10O	5	134.2	225	NA	2.56
B29	Pivalanilide	6625-74-7	C11H15NO	5	177.2	324	15.12	2.31
B30	Scienstab NA-11 / ADK Stab NA-11	85209-91-2	C29H42NaO4P	9.5	508.6	510	2.1	NA
B31	Triethyl phosphate	78-40-0	C6H15O4P	0	182.2	216	-9.1	1.08
B32	Kesscoflex TRA	102-76-1	C9H14O6	3	218.2	258	-6.5	-0.24
B33	Triethyl citrate	77-93-0	C12H20O7	3	276.3	294	NA	0.1
B34	2,2,4-Trimethyl-1,3-pentanediolediisobutyrate	6846-50-0	C16H30O4	2	286.4	380	NA	4.7
B35	Methyl oleate	112-62-9	C19H36O2	2	296.5	219	NA	7.6
B36	Isopropyl palmitate	142-91-6	C19H38O2	1	298.5	342	NA	8.2
B37	Diphenyl terephthalate	1539-04-4	C20H14O4	14	318.3	496	NA	4.12
B38	DEHS(Atrazine-desisopropyl-2-hydroxy)	7313-54-4	C5H9N5O	4	155.2	267	7.53±0.70	-0.16
B39	Tributyl citrate	77-94-1	C18H32O7	3	360.5	325	11.30±0.29	4.32
B40	Diisooctyl phthalate	27554-26-3	C24H38O4	6	390.6	235	NA	8.5
B41	Palatinol® DOTP	6422-86-2	C24H38O4	11	390.6	400	NA	9.55
B42	Acetyl n-tributyl citrate	77-90-7	C20H34O8	4	402.5	331	NA	3.3
B43	Plasthall® DOZ	2064-80-4	C25H48O4	2	412.7	428	NA	9.74
B44	2-Ethylhexyl sebacate	122-62-3	C26H50O4	2	426.7	212	NA	9.72
B45	Plasthall® DINP plasticizer	28553-12-0	C26H42O4	6	418.6	463	NA	9.6

GC Chemical Master List and Associated Physicochemical Properties

Code	Trivial name/ acronym	CAS #	Empirical Formula	Double Bond Equivalents (DBE)	Mol. Wt (g/mol)	Boiling Point (°C)	pKa	logP
B46	Diisononyl cyclohexane 1,2-dicarboxylate ester	166412-78-8	C26H48O4	3	424.7	489	NA	8.9
B47	Diisodecyl adipate	27178-16-1	C26H50O4	2	426.7	428	NA	10.08
B48	Dicyclohexyl phthalate	84-61-7	C20H26O4	8	330.4	425.8±18.0	NA	5.76
B49	Citroflex® B-6	82469-79-2	C28H50O8	4	514.7	522	NA	11.17
B50	Tricapryl trimellitate	27251-75-8	C33H54O6	7	546.8	585	NA	12.8
B51	Bis(2-ethylhexyl) cyclohexane-1,2-dicarboxylate	84-71-9	C24H44O4	3	396.6	463.9±20.0	NA	9.96
B52	Tri(n-octyl, n-decyl) trimellitate	67989-23-5	C72H120O12	13	1178	583	NA	20.817
B53	Retarder AK	85-44-9	C8H4O3	7	148.1	284	2.97	2.07
B54	Benzotriazole	95-14-7	C6H5N3	6	119.1	450	1.6	1.34
B55	HBT	3411-95-8	C13H9NOS	10	227.3	402.2±47.0	8.21	4.53
B56	Tinuvin 326	3896-11-5	C17H18ClN3O	10	315.8	460.4±55.0	9.31±0.48	6.58
B57	Uvinul® 3008, UV 531, Chimassorb 81	1843-05-6	C21H26O3	9	326.4	457.9±30.0	7.59±0.35	7.36
B58	Tinuvin 328	25973-55-1	C22H29N3O	10	351.5	469.1±55.0	8.85±0.50	7.3
B59	Tinuvin 770	52829-07-9	C28H52N2O4	4	480.7	499.8±45.0	10.49±0.10	7.32
B60	Uvinul® 3000	131-56-6	C13H10O3	9	214.2	409.0±14.0	7.72±0.35	3.17
B61	Tinuvin® PED	2440-22-4	C13H11N3O	10	225.3	272	8.15±0.43	2.73
B62	2-(2-Hydroxy-5-tert-octylphenyl)benzotriazole	3147-75-9	C20H25N3O	10	323.4	471.8±55.0	8.07±0.45	7.29
B63	BLS® 234 / 2-(2-Hydroxy-3,5-di(1,1-dimethylbenzyl)phenyl)benzotriazole	70321-86-7	C30H29N3O	18	447.6	589.3±60.0	9±0.10	9.21
B64	Accelerator ETU-22 PM	96-45-7	C3H6N2S	2	102.1	148.3±23.0	15.01±0.20	-0.66
B65	PFDA	335-76-2	C10HF19O2	1	514.1	219	0.52±0.10	9.53
B66	2-Ethylhexanol	104-76-7	C8H18O	0	130.2	184	15.06	2.82
B67	Lauro lactam	947-04-6	C12H23NO	2	197.3	315	16.91±0.20	3.34
B68	Tetradecane	629-59-4	C14H30	0	198.4	253	NA	5.7
B69	benzoyl isopropanol	7473-98-5	C10H12O2	5	164.2	80-81	13.23±0.29	1.13
B70	alpha-Cumyl alcohol	617-94-7	C9H12O	4	136.2	202	14.49±0.29	1.73

GC Chemical Master List and Associated Physicochemical Properties

Code	Trivial name/ acronym	CAS #	Empirical Formula	Double Bond Equivalent (DBE)	Mol. Wt (g/mol)	Boiling Point (°C)	pKa	logP
B71	1-Dodecene	112-41-4	C ₁₂ H ₂₄	1	168.3	213	NA	6.62
B72	Dodecylbenzenesulfonic acid	27176-87-0	C ₁₈ H ₃₀ O ₃ S	4	326.5	82	0.7	6.47
B73	Cyanox [®] LTDP	123-28-4	C ₃₀ H ₅₈ O ₄ S	2	514.8	580.8±35.0	NA	12.88
B74	Dioxitol	111-90-0	C ₆ H ₁₄ O ₃	0	134.2	202	14.37±0.10	-0.62