

ULTRAVIOLET COLLECTION

1980 CUMULATIVE LOCATOR INDEX



Sadtler Research Laboratories

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Sadtler Research Laboratories

ULTRAVIOLET SPECTRA LOCATOR

Ultraviolet spectra are a very useful analytical tool in illustrating important structural features and identifying unknown compounds. The spectroscopist frequently requires comparison spectra of known compounds for evaluation and it is to this end that the Sadtler Standard Ultraviolet Locator has been devised. Using the Locator it is possible to rapidly retrieve those spectra which most closely resemble an unknown spectrum. The retrieval method is based upon the wavelength location and absorptivity of the peaks in the ultraviolet spectra.

The Locator consists of up to five pairs of columns containing the spectral information; the sixth column shows the total number of absorption peaks exhibited in the region 200 - 350 $m\mu$ (some into the visible region), followed by the Sadtler spectrum serial number (both infrared and ultraviolet). The last column headed 'NAB' indicates whether the corresponding data was obtained from a spectrum determined in a neutral (N), acidic (A) or basic (B) medium. Since many compounds possessing ionizable functional groups exhibit spectral shifts and changes in absorptivity dependent on the pH of the solvent system, it is desirable to have this information as a further means of locating an unknown spectrum. It is also evident that often more than one spectrum will fulfill the requirements exacted by an unknown. The purpose of the Locator is to minimize the number of spectra to be examined for comparison purposes, it should not be considered as an absolute identification in itself. Similarly the infrared spectrum number is included in the Locator to provide further confirmation of unknown compounds if such information is required.

The Locator relies principally upon the first five pairs of columns for its operation. The first four digits of the first column pair denote the position of the peak of maximum absorption (highest absorptivity) to the nearest one half $m\mu$. The second set of four digits within the first column gives the value of the absorptivity (a) of that peak. To facilitate the use of the Locator with unknown compounds the absorptivity rather than the molar absorptivity has been used. The absorptivity has been calculated from.

$$a = \frac{A}{bC}$$

where

a	=	absorptivity
A	=	absorbance (also known as optical density or extinction)
b	=	optical path length in cm
C	=	concentration in grams per liter

In order to convert values of absorptivity (a) to molar absorptivity (ϵ) simply multiply by the molecular weight of the compound.

The entries in column pairs 2 through 5 have the same designation as the first column pair and are arranged in order of descending absorptivity. If there are less than five column pairs for a spectrum entry this indicates that the compound exhibits fewer than five absorption peaks in the 200 - 350 $m\mu$ range. Should all five column pairs be filled then the compound has five or more peaks in the 200 - 350 $m\mu$ region and the total number of peaks is given in the column labelled "PEAKS." The arbitrary decision to include specified values for a maximum of five peaks was made following a survey of the complete Sadtler Ultraviolet Spectra collection which showed that less than 10% of the spectra exhibited more than five peaks.

There are two methods of locating unknown spectra for comparison. Firstly, comparing on λ values only taking the λ values of the five strongest peaks without calculating the absorptivities. This method gives a rapid preliminary screening for possible matching spectra. The second and more precise method entails the calculation of absorptivity values and more detailed searching for spectra which match on both wavelength and absorptivity values.

During the searching procedure it is advisable to look at spectra within $\pm 0.5 \text{ m}\mu$ if an exact match cannot be found, this allows for instrument variation.

The example shown below illustrates the composition of the Ultraviolet Locator. On the following page a worked example of an actual spectrum is illustrated.

COLUMN PAIR NO.					NO. OF PEAKS IN ENTIRE SPECTRUM				SADTLER INFRARED SERIAL NO.				
1	2	3	4	5	PEAKS	IR NO	UV NO	NAB					
67.0	3.600	274.5	3.300		2	24241	8510	N					
67.0	2.550	274.5	2.300		2	41700	19099	B					
67.0	4.000	274.5	3.850		2	41700	19099	N					
67.0	1.519	274.5	1.325		2	46313	24221	B					
67.0	1.500	274.5	1.450		2	50628	26099	N					
67.0	4.400	274.5	3.850		2	53710	28298	B					
67.0	1.920	274.5	1.860	259.0	1.840	3	29804	12388	N				
67.0	2.083	275.0	1.736			2	19686	7806	N				
67.0	2.900	275.0	2.750			2	41265	18941	N				
67.0	1.908	275.0	1.686	259.0	1.464	4	6010	1694	N				
67.0	1.960	275.0	1.840	260.0	1.780	5	1545	444	N				
67.0	4.800	275.0	4.700	261.0	3.800	3	45697	23279	N*				
67.0	4.213	275.0	3.672	261.0	2.754	4	230	87	N				
67.0	20.89	275.0	18.65	307.5	11.94	4	30150	12645	B				

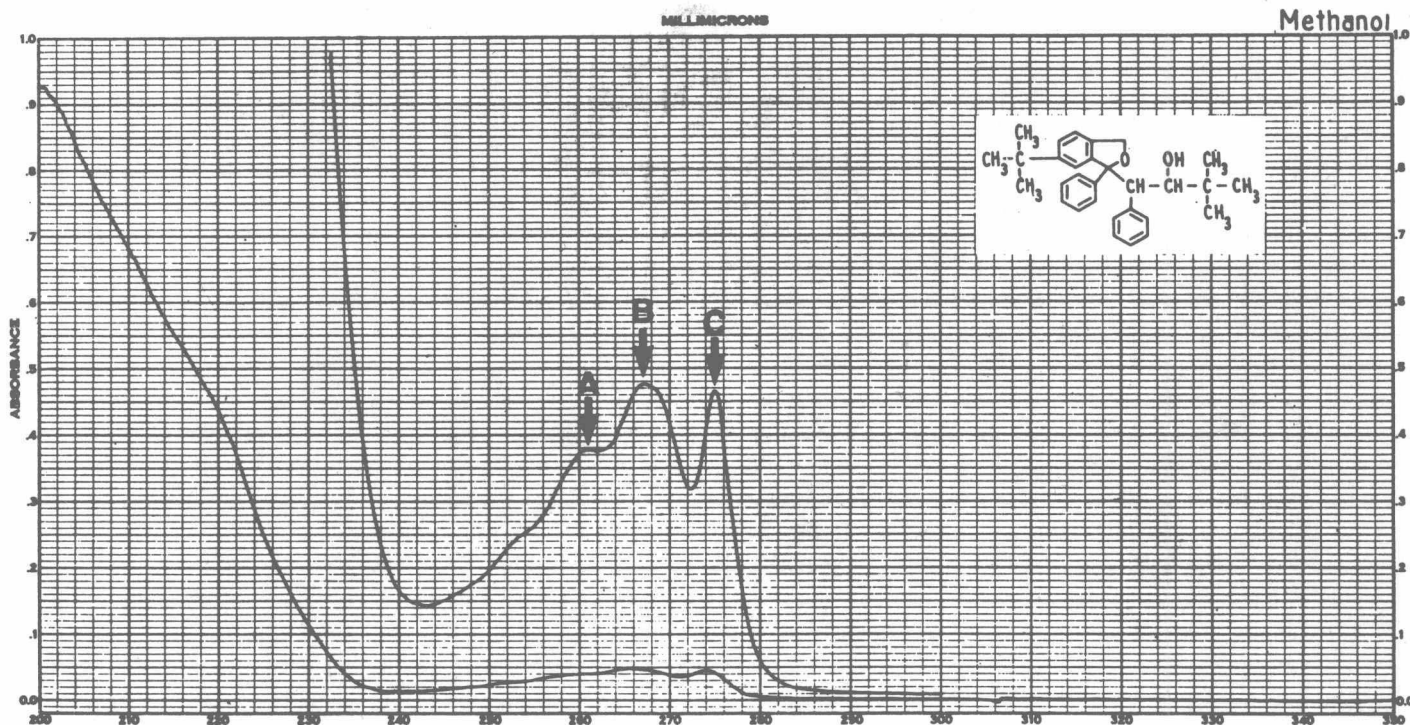
SADTLER ULTRAVIOLET
SERIAL NO.

SOLUTION MEDIUM
(ACID, BASE, NEUTRAL)

max -- ABSORPTIVITY
OR COLUMN PAIR NO. 1

EXAMPLE

1. Examine the spectrum (see illustration below) for all maxima and list them.
2. Calculate the absorptivity for each peak using the equation:
$$a = \frac{A}{bc}$$
3. Arrange the peak data in sequence according to decreasing absorptivity, listing both the $\lambda_{\max}$ and absorptivity values. This sequence will indicate which column pairs the data will fall into in the Locator.
4. Compare the data obtained from No. 3 above with the Locator, bearing in mind that the Locator is arranged according to increasing value of $\lambda_{\max}$.



Absorption Maxima	Absorptivity	Column Pair No.
$\lambda_{\max}$ (m μ)	a	
A •261.0	3.800	3
B •267.0	4.800	1
C •275.0	4.700	2

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NAME	PRISM	GRATING	UV	NMR	C-13
PROPANE, 2-NITRO-, BENZOYL CHLORIDE	1	1	1 N	13155	1601
ANILINE, N,N-DIMETHYL-, ETHANE, NITRO-, BENZYL CHLORIDE	3	5402	2 N	3147	1
TOLUENE, A-CHLORO-, 2-PICOLINE	6	4	3 NA	1	2
O-XYLENE	7	5	4 N	2	402
BENZENE, NITRO-, PYRIDINE	8	6	5 N	3	3
PHOSPHORIC ACID, TRI-M-TOLYL ESTER	8	6	5 N	3	3
M-TOLYL PHOSPHATE	9	7	6 N	566	403
PTHALIC ACID, BIS/2-METHOXYETHYL/ESTER	11	9	7 N	10199	4
PTHALIC ACID, BIS/2-BUTOXYETHYL/ESTER	12	10	8 N	4	1401
4-PICOLINE	15	12	9 N	10200	1201
3-PICOLINE	20	8002	10 N B	301	1604
P-CRESOL	20	8002	10 N B	301	1604
BENZENE, CHLORO-, PHOSPHONOTHIOIC ACID, PHENYL-, O,O-DIPHENYL ESTER	23	14	11 N	1120	6
ISOBENZOFURAN, 1,3-DIHYDRO-1,3-DIOXO-	26	16	12 N	1399	1607
ISOBENZOFURAN, 1,3-DIHYDRO-1,3-DIOXO-	31	17	13 N	889	8
1,3-ISOBENZOFURANDIONE	32	18	14 N	890	9
1,3-ISOBENZOFURANDIONE	33	8005	15 N	9491	1608
PTHALIC ANHYDRIDE	34	19	16 N	714	1402
PTHALIC ANHYDRIDE	38	41004P	17 NAB		
CYCLOHEXANONE, 4-METHYL-, PROPANE, 1-NITRO-, 2-PENTANONE, 4-METHYL-, 2-NAPHTHYLAMINE	39	21002	18 N	10133	
2-NAPHTHYLAMINE K	8656	21002	18 N	10133	
PHOSPHONIC ACID, PHENYL-, DIALLYL ESTER	39	21002	18 N	10133	
SULFAMERAZINE	8656	21002	18 N	10133	
SULFAMERAZINE K	39	21002	18 N	10133	
SULFANILAMIDE, N<1-/4-METHYL-2-PYRIMIDINYL/-	8656	21002	18 N	10133	
ACETYSALICYLIC ACID	42	24506	19 N	8	404
ASPIRIN	43	22	20 N	10192	
SALICYLIC ACID, ACETATE	44	23	21 N	10201	405
PHENYL SULFONE	46	33001	22 N	25001	
PYRIMIDINE, 4,6-DICHLORO-, ACETIC ACID, DIFLUORO-, METHYL ESTER	9640	33001	22 N	25001	
METHANE, NITRO-, DIPHENYLAMINE	47	41005P	23 N		
TRYPTOPHAN, N-CARBOXY-, N-BENZYL ESTER, L-	49	41006P	24 N	8370	4605
BENZENE, 1-CHLORO-2-ETHYL-, BENZENE, M-DINITRO-, HOMATROPINE, METHOBROMIDE	9024	41006P	24 N	8370	4605
HOMATROPINIUM BROMIDE, 8-METHYL-, TROPINE, MANDELATE, METHOBROMIDE	49	41006P	24 N	8370	4605
PHENOL, P-ETHOXY-, GUAIACOL	51	32501	25 N	18001	4607
PHENOL, O-METHOXY-, TOLUENE, O-CHLORO-, 3,4-PYRIDINEDIMETHANOL, 5-HYDROXY-6-METHYL-, HYDROCHLORIDE	51	32501	25 N	18001	4607
3,4-PYRIDINEDIMETHANOL, 5-HYDROXY-6-METHYL-, HYDROCHLORIDE	51	32501	25 N	18001	4607
PYRIDOXINE, HYDROCHLORIDE	53	24	26 N	17333	4001
PYRIDOXINE, HYDROCHLORIDE	55	8008	27 N	7335	4402
PYRIDOXOL, HYDROCHLORIDE	56	41008P	28 N	11478	
VITAMIN B6, HYDROCHLORIDE	61	25	29 N	9146	4002
VITAMIN B6, HYDROCHLORIDE	68	8009	30 N	11	17
4-HEPTANONE, 2,6-DIMETHYL-, 4-HEPTANONE, 2,6-DIMETHYL-, ACETOACETIC ACID, ETHYL ESTER	1328	8142	31 N	23014	5003
MESITYL OXIDE	79	26	32 N	1111	1612
3-PENTEN-2-ONE, 4-METHYL-, 2-FURALDEHYDE	81	27	33 N	10134	4004
FURFURAL	83	21004	34 N	10238	
FURFUROLE	83	21004	34 N	10238	
ACETONE, ACETONYL-, 2,5-HEXANEDIONE	83	21004	34 N	10238	
2-CYCLOHEXEN-1-ONE, 3,5,5-TRIMETHYL-, ISOPHORONE	85	24508	35 N	12	26
	90	8013	36 N B	3149	805
	90	8013	36 N B	3149	805
	91	29	37 N	13	1614
	92	30	38 N B	17264	5001
	8085	30	38 N B	17264	5001
	92	30	38 N B	17264	5001
	8085	30	38 N B	17264	5001
	92	30	38 N B	17264	5001
	8085	30	38 N B	17264	5001
	99	31	39 N	10135	806
	6230	31	39 N	10135	806
	101	32	40 N	10321	1616
	109	18001	41 N	13213	
	109	18001	41 N	13213	
	113	35	42 N	10203	1618
	113	35	42 N	10203	1618
	113	35	42 N	10203	1618
	121	15015	43 N	2709	34
	121	15015	43 N	2709	34
	122	36	44 N	7311	4612
	122	36	44 N	7311	4612

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NAME	PRISM	GRATING	UV	NMR	C-13
2-FURANMETHANOL	124	10765	45 N	17032	1619
FURFURYL ALCOHOL	124	10765	45 N	17032	1619
2-FURANCARBOXYLIC ACID	126	38	46 N B	10235	4614
2-FUROIC ACID	126	38	46 N B	10235	4614
PYROMUCIC ACID	126	38	46 N B	10235	4614
ETHANE, 2,2-BIS(P-CHLOROPHENYL)-	127	15014	47 N	15	4401
1,1,1-TRICHLORO-					
PENICILLIN G, S,S-DIOXIDE,	130	15251	48 N	6908	
METHYL ESTER					
PENICILLIN, BENZYL-, S,S-DIOXIDE,	130	15251	48 N	6908	
METHYL ESTER					
4-THIA-1-AZABICYCLO[3.2.0]HEPTANE-2-	130	15251	48 N	6908	
CARBOXYLIC ACID, 3,3-DIMETHYL-7-OXO-6-					
/2-PHENYLACETAMIDO-, 4,4-DIOXIDE,					
METHYL ESTER					
PHENETHYLAMINE, DL-A-METHYL-,	134	41016P	49 N		
SALICYLIC ACID, 5-SULFO-,	137	29551	50 N	16001	4617
O-TOLUIC ACID	139	41	51 N B	17	4618
M-TOLUIC ACID	140	42	52 N B	18	4619
MERCURY, /ACETATO-PHENYL-,	141	21005	53 N	10205	4803
MERCURY, ACETOXYPHENYL-,	141	21005	53 N	10205	4803
FLUOREN-2-AMINE	145	233	54 N	18667	
2-FLUORENAMINE	145	233	54 N	18667	
BENZENE, P-DICHLORO-	146	44	55 N	715	37
BENZOIC ACID, P-CHLORO-,	147	45	56 N B	10266	4621
BENZOIC ACID, P-CHLORO-, /KBR/	11200	45	56 N B	10266	4621
GLYCINE, N-/N-CARBOXYVALYL-,	1371	8151	57 N		
N-BENZYL ETHYL ESTER, DL-,					
ACETAMIDE, N-METHYL-2-PHENYL-,	151	46	58 N	6359	4622
FLAVONE, 3-/6-B-L-RHAMNOPYRANO-	152	21006	59 N		
SIDO-D-GLUCOPYRANOSYL/OXY-/3PR,4PR,5,7-					
TETRAHYDROXY-, DIHYDRATE					
FLAVONE, 3-/6-B-L-RHAMNOPYRANO-	11488	21006	59 N		
SIDO-D-GLUCOPYRANOSYL/OXY-/3PR,4PR,5,7-					
TETRAHYDROXY-, DIHYDRATE					
QUERCETIN, 3-RUTINOSIDE, DIHYDRATE	152	21006	59 N		
QUERCETIN, 3-RUTINOSIDE, DIHYDRATE	11488	21006	59 N		
RUTIN	152	21006	59 N		
RUTIN	11488	21006	59 N		
BENZENE, P-DIHYDROXY-,	153	47	60 N	10350	38
BENZENE, P-DIHYDROXY-,	13206	47	60 N	10350	38
P-BENZENEDIOL	153	47	60 N	10350	38
P-BENZENEDIOL	13206	47	60 N	10350	38
HYDROQUINOL	153	47	60 N	10350	38
HYDROQUINOL	13206	47	60 N	10350	38
HYDROQUINONE	13206	47	60 N	10350	38
HYDROQUINONE	153	47	60 N	10350	38
QUINOL	153	47	60 N	10350	38
QUINOL	13206	47	60 N	10350	38
ANILINE, N-/2-NAPHTHYL-,	155	48	61 N	10206	4804
2-NAPHTHYLAMINE, N-PHENYL-,	155	48	61 N	10206	4804
BENZYL ALCOHOL	157	985	62 N	9374	1804
METHANOL, PHENYL-,	157	985	62 N	9374	1804
A-TOLUENOL	157	985	62 N	9374	1804
ACETANILIDE	160	49	63 N	5235	4201
ACETIC ACID, PHENYL-, METHYL ESTER	165	4764	64 N	19	40
CYCLOHEXANONE	166	51	65 N	10208	409
CINNAMIC ACID, METHYL ESTER	167	52	66 N	20	4624
CYCLOPENTANONE	171	55	67 N	1195	42
THIOFURAN	172	29684	68 N	10285	1202
THIOPHENE	172	29684	68 N	10285	1202
2-THIOPHENECARBOXALDEHYDE	174	56	69 N	10165	43
THIOPHENE-2-CARBOXYLIC ACID	176	963	70 N B	523	4805
2-THIOPHENECARBOXYLIC ACID	176	963	70 N B	523	4805
THIOPHENE, 2-NITRO-,	177	57	71 N	31622	
ANILINE, N-/1-NAPHTHYL-,	179	58	72 N	21	4628
1-NAPHTHYLAMINE, N-PHENYL-,	179	58	72 N	21	4628
TOLUENE, M-NITRO-,	183	61	73 N	22	2002
CINNAMYL ALCOHOL	184	8018	74 N	23	46
2-PROPEN-1-OL, 3-PHENYL-,	184	8018	74 N	23	46
CINCHONIC ACID, 6-METHYL-2-	186	15261	75 N	6276	4629
PHENYL-, ETHYL ESTER					
CINCHONIC ACID, 6-METHYL-2-	11645	15261	75 N	6276	4629
PHENYL-, ETHYL ESTER					
NEOCINCHOPHEN	186	15261	75 N	6276	4629
NEOCINCHOPHEN	11645	15261	75 N	6276	4629
NOVATOPHAN	186	15261	75 N	6276	4629
NOVATOPHAN	11645	15261	75 N	6276	4629
8-QUINOLINOL	187	63	76 N	24	4630
BENZENE, ETHOXY-,	192	4826	77 N	26	4202
PHENETOLE	192	4826	77 N	26	4202
STYRENE, A-METHYL-,	195	8020	78 N	V 232	50
COUMALIC ACID	203	15019	79 N	6491	4633

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NAME	PRISM	GRATING	UV	NMR	C-13
GLUTACONIC ACID, 4-/HYDROXY-METHYLENE/-, D-LACTONE	203	15019	79 N	6491	4633
2H-PYRAN-5-CARBOXYLIC ACID, 2-OXO-, ANILINE, M-NITRO-, PENICILLIN G	203 205 206	15019 70 41022P	79 N 80 NA 81 N	6491 13454	4633 5801
PENICILLIN, BENZYL-, 4-THIA-1-AZABICYCLO[3.2.0]HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-7-OXO-6-/2-PHENYLACETAMIDO/-, FURAN, 2-METHYL-, SYLVAN	206 206 210 210 216	41022P 41022P 28978 28978 72	81 N 81 N 82 N 82 N 83 NA	81 N 81 N 6662 6662 716	411 411 412
ANILINE, N,N-DIETHYL-, CARBONIC ACID, PHENYL ESTER, DIESTER WITH DIETHYLENE GLYCOL	224	41027P	84 N		
DIETHYLENE GLYCOL, BIS/PHENYL CARBONATE/	224	41027P	84 N		
TOLUENE, O-CHLORO-A,A,A-TRIFLUORO-, TOLUENE, P-CHLORO-A,A,A-TRIFLUORO-, TOLUENE, M-CHLORO-A,A,A-TRIFLUORO-, BENZOTRIFLUORIDE	225 226 230 232	74 75 15021 28979	85 N 86 N 87 N 88 N	10137 1177 18328 6569	2401 2004 4807 1811
TOLUENE, A,A,A-TRIFLUORO-, ACETONE	232 233	28979 77	88 N 89 N	6569 9288	1811 413
ACETONE	6309	77	89 N	9288	413
METHYL KETONE	6309	77	89 N	9288	413
2-PROPANONE	233	77	89 N	9288	413
2-PROPANONE	6309	77	89 N	9288	413
1-NAPHTHOIC ACID, 2-HYDROXY-, 1-NAPHTHOIC ACID, 2-HYDROXY-	234 13209	78 78	90 N B 90 N B	13433 13433	4634 4634
AS-TRIAZINE, 5,6-DIMETHYL-3-PHENYL-, TOLUENE, M-NITRO-A,A,A-TRIFLUORO-, TOLUENE, 4-CHLORO-3-NITRO-A,A,A-TRIFLUORO-, BENZENE, VINYL-, CINNAMENE	235 236 238 241 241	41029P 8022 80 81 81	91 N 92 N 93 N B 94 N 94 N		
PHENETHYLENE	241	81	94 N	6408	4006
STYRENE	241	81	94 N	6408	4006
STYROL	241	81	94 N	6408	4006
BENZENE, ISOPROPYL-, CUMENE	242 242	8023 8023	95 N 95 N	10183 10183	58 58
BICYCLO[2.2.1]HEPTAN-2-ONE, 1,7,7-TRIMETHYL-, 2-CAMPHANONE	244 244	15264 15264	96 N 96 N	30 30	4635 4635
CAMPHOR	244	15264	96 N	30	4635
CAMPHOR K	9598	15264	96 N	30	4635
BENZENE, ETHYL-, BENZENE, SEC-BUTYL-, ETHANOL, 2-PHENOXY-, ETHANOL, 2-/P-SEC-BUTYLPHENOXY/-, BENZOIC ACID, O-CHLORO-, BENZOIC ACID, O-CHLORO-, /KBR/	246 247 248 249 251 11198	82 83 84 15024 85 85	97 N 98 N 99 N 100 N 101 N B 101 N B	V 505 * 155 10211 6663 10212 10212	1621 60 61 1814 4808 4808
P-ACETOPHENETIDIDE	252	4849	101 N	V 267	4636
PHENACETIN	252	4849	102 N	V 267	4636
M-CRESOL, 6-TERT-BUTYL-, ETHANOL, 2-/P-TERT-BUTYLPHENOXY/-, BENZOIC ACID, 2,4-DIHYDROXY-, TRIHYDRATE	257 259 260	89 15026 90	103 N B 104 N 105 N B	525 6664 9527	2005 1816 5002
BENZOIC ACID, 2,4-DIHYDROXY-, TRIHYDRATE	13212	90	105 N B	9527	5002
B-RESORCYLIC ACID, TRIHYDRATE	260	90	105 N B	9527	5002
B-RESORCYLIC ACID, TRIHYDRATE	13212	90	105 N B	9527	5002
M-CRESOL, 4,6-DI-TERT-BUTYL-, BUTYRIC ACID, 2-PHENYL-, ETHYL ESTER	262 263	4896 15027	106 N 107 N	10197 6641	
BENZENE, O-DIHYDROXY-, PYROCATECHOL	268 268	29687 29687	108 N 108 N	17034 17034	64 64
PROPIOPHENONE	272	94	109 N	34	66
DIPHENETHYLAMINE	277	15028	110 N	6917	67
INDOLE, 3,3*-METHYLENEDI-, PHENOL, PENTACHLORO-, PHENETHYLAMINE	278 279 280	8026 96 8027	111 N 112 N 113 N		
ANILINE, N-BENZYL-N-ETHYL-, BENZYLAMINE, N-ETHYL-N-PHENYL-, MESITOL	288 288 295	24512 24512 8029	114 N 114 N 115 N	1178 1178 8657	1820 1820 6401
PHENOL, 2,4,6-TRIMETHYL-, HEMIMELLITENOL	295 296	8029 36751	115 N 116 N	8657 6013	6401 4645
PHENOL, 3,4,5-TRIMETHYL-, BENZENESULFONAMIDE, P-AMINO-, DESEPTYL	296 301 301	36751 102 102	116 N 117 NAB 117 NAB	6013 9685 9685	4645 4009 4009
PRONTOSIL ALBUM	301	102	117 NAB	9685	4009
PRONTYLIN	301	102	117 NAB	9685	4009
SULFANILAMIDE	301	102	117 NAB	9685	4009
ACETONITRILE, /5-ACETYL-2-ETHOXY-PHENYL/-, 9/79	305	41035P	118 N		

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NAME	PRISM	GRATING	UV	NMR	C-13
SULFANILAMIDE, N<1-/2-THIAZOLYL/-,	311	106	119 N	6666	4809
SULFATHIAZOLE	311	106	119 N	6666	4809
SULFIDE, METHYL PHENYL,	315	33944	120 N	19831	71
PHENYL SULFIDE	320	108	121 N	39	75
PHENOTHIAZINE	321	109	122 N	9237	4403
PHENOTHIAZINE	3669	109	122 N	9237	4403
10H-PHENOTHIAZINE	321	109	122 N	9237	4403
THIODIPHENYLAMINE	321	109	122 N	9237	4403
ANEURINE	324	18003	123 N	13482	4404
THIAMINE, HYDROCHLORIDE	324	18003	123 N	13482	4404
THIAZOLIUM CHLORIDE, 3-/4-AMINO-2-	324	18003	123 N	13482	4404
METHYL-5-PYRIMIDINYL/METHYL-/5-/2-					
HYDROXYETHYL-/4-METHYL-, HYDROCHLORIDE					
VITAMIN B1, HYDROCHLORIDE	324	18003	123 N	13482	4404
ETHYL DISULFIDE	325	36752	124 N	17036	419
BENZOIC ACID, O-MERCAPTO-,	327	15032	125 N	6668	
2-NAPHTHALENETHIOL	331	21007	126 N	17037	4405
BENZOYL PEROXIDE	332	36004	127 N	7604	
PHTHALIC ACID, BIS/2-ETHYLBUTYL/	335	41038P	128 N		
ESTER					
ANILINE, N,N-DIMETHYL-P-/A,A,A-	343	41039P	129 N	10418	
TRIFLUORO-M-TOLYL/AZO/-,					
ANILINE, N,N-DIMETHYL-P-/P-	344	15034	130 N	7532	
FLUOROPHENYL/AZO/-,					
ANILINE, N,N-DIMETHYL-P-/O-	345	15035	131 N	7533	
FLUOROPHENYL/AZO/-,					
ANILINE, N,N-DIMETHYL-P-/O-	346	15266	132 N	7534	4406
TOLYL/AZO/-,					
ANILINE, N,N-DIMETHYL-P-/O-	346	44688P	132 N	7534	4406
TOLYL/AZO/-,					
ANILINE, N,N-DIMETHYL-P-/O-	8093	44688P	132 N	7534	4406
TOLYL/AZO/-,					
ANILINE, N,N-DIMETHYL-P-/O-	8093	15266	132 N	7534	4406
TOLYL/AZO/-,					
ANILINE, N,N-DIMETHYL-P-/PHENYL-	347	21685	133 N	10351	4407
AZO/-,					
ANILINE, N-METHYL-P-/PHENYL/AZO/-,	348	15267	134 N	18329	4408
ANILINE, N,N-DIMETHYL-P-/P-	349	15036	135 N	7535	
TOLYL/AZO/-,					
AZOBENZENE	350	115	136 N	43	79
BENZENE/AZOBENZENE	350	115	136 N	43	79
ANILINE, N-METHYL-P-/M-TOLYL/AZO/-,	352	15268	137 N	10742	
M-TOLUIDINE, N,N-DIMETHYL-P-	354	15269	138 N	7536	4409
/PHENYL/AZO/-,					
M-TOLUIDINE, N,N-DIMETHYL-P-	8094	15269	138 N	7536	4409
/PHENYL/AZO/-,					
2-PENTANONE, 4-HYDROXY-4-METHYL-,	356	116	139 N	303	2807
ANILINE, N,N-DIMETHYL-P-/M-	357	15037	140 N	7537	4410
FLUOROPHENYL/AZO/-,					
ANILINE, P-/P-CHLOROPHENYL/AZO/-	358	15038	141 N	7538	
N,N-DIMETHYL-,					
ANILINE, P-/PHENYL/AZO/-,	359	8032	142 NA	13484	4411
C.I. SOLVENT YELLOW 1	359	8032	142 NA	13484	4411
ANILINE, N,N-DIMETHYL-P-/M-	360	15039	143 N	7539	4412
TOLYL/AZO/-,					
ANILINE, P-/O-CHLOROPHENYL/AZO/-	361	15040	144 N	7540	4413
N,N-DIMETHYL-,					
ANILINE, N,N-DIMETHYL-P-/A,A,A-	364	41041P	145 N	7541	
TRIFLUORO-O-TOLYL/AZO/-,					
ACETAMIDE, /5-ACETYL-2-METHOXY-	369	41043P	146 N		
PHENYL/-,					
PEROXIDE, BIS/O-CARBOXYBENZOYL/,	370	41044P	147 N		
UREA, AMIDINO-, PHOSPHATE	371	15041	148 NAB		
BENZOFURO/4,5-B//1/BENZOPYRANO-	373	21008	149 N	10340	6201
/4,3-E/PYRAN-6/6AH/-ONE, 8,9-DIMETHOXY					
2-ISOPROPENYL-1,2,12,12A-TETRAHYDRO-,					
BENZOPYRANO/3,4-B/FURO/2,3-H//1/-	373	21008	149 N	10340	6201
BENZOPYRAN-6/6AH/-ONE, 8,9-DIMETHOXY-2					
ISOPROPENYL-1,2,12,12A-TETRAHYDRO-,					
PHTHALIC ACID, DIETHYL ESTER	375	117	150 N	705	82
PHLOROGLUCINOL, METHYL-,	379	8033	151 N	8135	4415
ALANINE, N-/CHLOROACETYL-/3-	1548	8164	152 N	567	6430
PHENYL-, L-/PLUS/-,					
DIPHENYLAMINE, N-NITROSO-,	390	21687	153 N	10374	4011
BENZENESULFONYL CHLORIDE	415	118	154 N	3150	90
BENZENE, METHYL-,	419	119	155 N	V 157	91
TOLUENE	419	119	155 N	V 157	91
ETHANOL, 2-/4-CHLORO-2-NITRO-	420	41069P	156 N		
PHENOXY/-,					
DIPHENYLAMINE, 4-ISOPROPOXY-,	426	15045	157 N		
BENZOIC ACID, THIO-, S-BENZYL ESTER	427	28507	158 N	13154	
TRYPTOPHAN, N-BENZOYL-, L-,	428	41071P	159 N		
ACETONITRILE, 3,4-DIMETHOXYPHENYL-,	431	24514	160 N	10267	4418

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2H-TETRAZOLIUM CHLORIDE, 2,3,5-TRI-PHENYL-, K	10531	15278	193 N	6281	
P-CRESOL, 2,6-BIS/1,1,3,3-TETRA-METHYLBUTYL/-	565	15279	194 N	6461	
BIGUANIDE, 1-PHENYL-, HYDROCHLORIDE	567	15059	195 NAB	27504	
BIGUANIDE, 1-PHENYL-, HYDROCHLORIDE	8574	15059	195 NAB	27504	
P-DIOXINO/2,3-F/QUINOLINE, 2,3-DI-HYDRO-6-/5-/ISOPROPYLAMINO/PENTYL-AMINO/-, PHOSPHATE	570	41100P	196 N		
QUINOLINE, 5,6-/ETHYLENEDIOXY/-8-/5-/ISOPROPYLAMINO/PENTYLAMINO/-, PHOSPHATE	570	41100P	196 N		
ACETAMIDE, 2-/5-ACETYL-2-/ISO-PENTYLOXY/PHENYL/-	572	41102P	197 N		
BENZENE	579	136	198 N	3429	425
BENZOL/E/	579	136	198 N	3429	425
BENZOIC ACID, 3,4-DICHLORO-, BENZOIC ACID, 2,4-DICHLORO-,	583	137	199 N B	8055	
5-BENZOFURANACRYLIC ACID, 6-HYDROXY-B-METHYL-, D-LACTONE	585	138	200 N	3340	6403
7H-FURO/3,2-G/1/BENZOPYRAN-7-ONE, 5-METHYL-	597	41116P	201 N		
5-BENZOFURANPROPIONIC ACID, 2,3-DI-HYDRO-6-HYDROXY-B-METHYL-, D-LACTONE	600	41118P	202 NAB		
7H-FURO/3,2-G/1/BENZOPYRAN-7-ONE, 5-METHYL-2,3,5,6-TETRAHYDRO-,	600	41118P	202 NAB		
TOLUENE, A,2,4-TRICHLORO-,	617	139	203 N	308	108
TOLUENE, A,A,A,4-TETRACHLORO-,	619	140	204 N	1181	109
BENZALDEHYDE, 2,4-DICHLORO-,	620	10845	205 N	3151	4657
TOLUENE, A,0-DICHLORO-,	621	141	206 N	1182	110
BENZALDEHYDE, P-CHLORO-,	624	8075	207 N	V 146	112
BENZALDEHYDE, O-CHLORO-,	625	8076	208 N	50	113
TOLUENE, A,4-DICHLORO-,	626	142	209 N	1183	114
TOLUENE, 3,4-DICHLORO-,	627	143	210 N	574	115
TOLUENE, 2,4-DICHLORO-,	628	144	211 N	1185	116
TOLUENE, P-CHLORO-,	629	145	212 N	51	117
TOLUENE, A,A,A,3,4-PENTACHLORO-,	631	146	213 N	1186	119
ACETIC ACID, /PENTACHLOROPHENOXY/-, METHYL ESTER	636	15281	214 N	6168	
ACETIC ACID, /2-NAPHTHYLOXY/-, METHYL ESTER	637	15061	215 N	6171	4811
ACETIC ACID, /2,3,4,6-TETRACHLORO-PHENOXY/-, ETHYL ESTER	638	15062	216 N	6172	
ACETIC ACID, /2,4,5-TRICHLORO-PHENOXY/-, ETHYL ESTER	639	15282	217 N	6173	4812
ACETIC ACID, /P-CHLOROPHENOXY/-, ETHYL ESTER	640	15063	218 N	6174	120
ACETIC ACID, /4-CHLORO-O-TOLYLOXY/-, ETHYL ESTER	642	41135P	219 N		
ACETIC ACID, /2,4-DICHLORO-PHENOXY/-, ETHYL ESTER	643	41136P	220 N		
BRUCINE, SULFATE, HEPTAHYDRATE	655	29321	221 N	3213	
BRUCINE, SULFATE, HEPTAHYDRATE	7453	29321	221 N	3213	
4,6-METHANO-6H,14H-INDOLO/3,2,1-IJ/OX-EPINO/2,3,4-DE/PYRROLO/2,3-H/QUINOLIN-14-ONE, 2,4A,5,5A,7,8,15,15A,15B,15C-DECAHYDRO-10,11-DIMETHOXY-, SULFATE, HEPTAHYDRATE	655	29321	221 N	3213	
GLUCOSE, PENTADIGALLATE	656	147	222 N		
TANNIC ACID	656	147	222 N		
3-INDOLEACETIC ACID	670	149	223 N	1198	4659
PHTHALIC ACID, DIISOCTYL ESTER	673	8082	224 N		
PHTHALIC ACID, DICYCLOHEXYL ESTER	37	3837	225 N	1199	124
PHTHALIC ACID, DICYCLOHEXYL ESTER	674	3837	225 N	1199	124
PHTHALIC ACID, DIOCTYL ESTER	675	8083	226 N	10218	125
PHOSPHORIC ACID, P-TOLYL ESTER	676	150	227 N	7013	
P-TOLYL PHOSPHATE	676	150	227 N	7013	
BENZENE, TERT-BUTYL-,	679	152	228 N	53	815
2-IMIDAZOLIN-4/OR5/-ONE, 5/OR4/-P-ETHOXYBENZYLIDENE/-1-HYDROXY-2-PHENYL-,	701	29129	229 N		
2-IMIDAZOLIN-5-ONE, 4-BENZYLIDENE-1-HYDROXY-2-PHENYL-,	703	41150P	230 N		
PROPIONIC ACID, 3-//2-BENZOTHAZOLYL/THIO/-	705	15070	231 N	6553	4661
HYDROQUINONE, METHYL-,	707	18404	232 N	9249	130
P-TOLUHYDROQUINONE	707	18404	232 N	9249	130
HYDROQUINONE, 2,5-DI-TERT-BUTYL-,	708	15071	233 N	7289	220
HYDROQUINONE, 2,5-DI-TERT-BUTYL-, M	1507	15071	233 N	7289	220
BENZENE, P-DIMETHOXY-,	710	156	234 N	56	131
BENZENE, P-DIETHOXY-,	711	157	235 N	309	432
PHENOL, P-AMINO-,	712	158	236 NAB	717	4663
P-BENZOQUINONE, 2,5-DI-TERT-BUTYL-,	713	159	237 N B	10316	4664
AS-TRIAZINE, 5,6-DIETHYL-3-PHENYL-,	714	41151P	238 N		

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HOMOERATRONITRILE	431	24514	160 N	10267	4418
NIACIN	434	120	161 NAB	14671	
NICOTINIC ACID	434	120	161 NAB	14671	
3-PYRIDINECARBOXYLIC ACID	434	120	161 NAB	14671	
M-PHENYLENEDIAMINE, DIHYDROCHLORIDE	459	29695	162 N B	3148	4426
2,5-FURANDIONE	462	8040	163 N	V 48	4427
MALEIC ANHYDRIDE	462	8040	163 N	V 48	4427
CYCLOHEXANOL, 2-PHENYL-,	468	126	164 N	10185	
BUTENDIOIC ACID, TRANS-,	472	127	165 N	4407	4650
1,2-ETHENEDICARBOXYLIC ACID, TRANS-,	472	127	165 N	4407	4650
FUMARIC ACID	472	127	165 N	4407	4650
CINCHONINIC ACID, 2-PHENYL-,	473	128	166 NAB	10217	4429
CINCHONINIC ACID, 2-PHENYL-,	11644	128	166 NAB	10217	4429
CINCHOPHEN	473	128	166 NAB	10217	4429
CINCHOPHEN	11644	128	166 NAB	10217	4429
4-QUINOLINECARBOXYLIC ACID, 2-PHENYL-,	473	128	166 NAB	10217	4429
4-QUINOLINECARBOXYLIC ACID, 2-PHENYL-,	11644	128	166 NAB	10217	4429
PHENOL, P-/BENZYLOXY/-,	474	15254	167 N	6552	98
PHENOL, 2,3,6-TRIMETHYL-,	475	33337	168 N	21134	813
BENZENEARSONIC ACID, P-HYDROXY-,	478	33338	169 N	6643	4430
2,5-PYRROLIDINEDIONE	482	129	170 N	6673	101
SUCCINIMIDE	482	129	170 N	6673	101
BARBITURIC ACID, 5-ETHYL-5-PHENYL-,	483	21015	171 N	6644	4431
PHENOBARBITAL	483	21015	171 N	6644	4431
DURENOL	486	15165	172 N	6015	4432
PHENOL, 2,3,5,6-TETRAMETHYL-,	486	15165	172 N	6015	4432
PHENOL, 2,4,6-TRI-TERT-BUTYL-,	488	130	173 N	707	
THEOPHYLLINE	493	24515	174 N B	13485	
XANTHINE, 1,3-DIMETHYL-,	493	24515	174 N B	13485	
CINCHONIDINE	502	131	175 NA	25874	
CINCHONIDINE	502	8554	175 NA	25874	
CINCHONIDINE	9521	131	175 NA	25874	
CINCHONIDINE	9521	8554	175 NA	25874	
CINCHONINE	502	8554	175 NA	25874	
CINCHONINE	502	131	175 NA	25874	
CINCHONINE	9521	8554	175 NA	25874	
CINCHONINE	9521	131	175 NA	25874	
4-QUINOLINEMETHANOL, A-/5-VINYL-2-QUINUCLIDINYL/-,	502	8554	175 NA	25874	
4-QUINOLINEMETHANOL, A-/5-VINYL-2-QUINUCLIDINYL/-,	502	131	175 NA	25874	
4-QUINOLINEMETHANOL, A-/5-VINYL-2-QUINUCLIDINYL/-,	9521	8554	175 NA	25874	
4-QUINOLINEMETHANOL, A-/5-VINYL-2-QUINUCLIDINYL/-,	9521	131	175 NA	25874	
ACETIC ACID, /3,4-DIMETHOXY-PHENYL/-,	506	132	176 N	10402	2809
ACETIC ACID, 3,4-DIMETHOXYPHENYL-,	11174	132	176 N	10402	2809
HOMOERATRIC ACID	506	132	176 N	10402	2809
BENZYL ALCOHOL, A-/1-/METHYLAMINO-/ETHYL/-,	520	33339	177 N		
EPHEDRINE	520	33339	177 N		
2,4-XYLENOL	521	15054	178 N	6016	104
PHENOL, P-TERT-BUTYL-,	522	133	179 N	47	1406
PHENOL, P-TERT-BUTYL-,	8111	133	179 N	47	1406
2-THIOPHENEPROPIONIC ACID, 8-OXO-, ETHYL ESTER	523	15055	180 N	10389	105
2-THIOPHENEPROPIONIC ACID, 8-OXO-, ETHYL ESTER	5831	15055	180 N	10389	
PHENOL, 2,6-DI-TERT-BUTYL-4-ETHOXY-,	525	15056	181 N	6458	
PHENOL, 2,6-DI-TERT-BUTYL-4-METHOXY-,	526	15276	182 N	6459	
PHENOL, 2-ISOBORNYL-,	528	41091P	183 N	10360	
P-CRESOL, 2,6-DIISOBORNYL-,	529	41092P	184 N		
P-CRESOL, 2-ISOBORNYL-,	530	41093P	185 N		
2,4-XYLENOL, 6-ISOBORNYL-,	532	24517	186 N	10361	
TRYPTOPHAN, N-ACETYL-, L-,	535	134	187 N		
BARBITURIC ACID, 5-BUTYL-5-/8-HYDROXYPHENETHYL/-,	536	41095P	188 N		
2,4-XYLENOL, 6-TERT-BUTYL-,	537	135	189 N	307	1407
4-PYRIMIDINOL, 2,5,6-TRIAMINO-, SULFATE, HYDRATE	856	8105	190 N		
4-PYRIMIDINOL, 2,5,6-TRIAMINO-, SULFATE, HYDRATE	856	8105	190 N		
P-CRESOL, 2-/1,1,3,3-TETRAMETHYL-BUTYL/-,	545	15057	191 N	6460	
2,4-XYLENOL, 6-/1,1,3,3-TETRAMETHYL-BUTYL/-,	546	41096P	192 N		
2H-TETRAZOLIUM CHLORIDE, 2,3,5-TRIPHENYL-,	560	15278	193 N	6281	

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CORTICOSTERONE, 11-DEOXY-, ACETATE	726	33342	239 N	27201	4816
PREGN-4-ENE-3,20-DIONE, 21-HYDROXY-, ACETATE	726	33342	239 N	27201	4816
SUCCINIMIDE, N-BENZYL-2-/BENZYL-NITROSAMINO/-, K	735	15072	240 N	7264	4665
SUCCINIMIDE, N-BENZYL-2-/BENZYL-NITROSOAMINO/-, K	11637	15072	240 N	7264	4665
ASPARAGINE, N<2-ACETYL-N-BENZYL-, ASPARAGINE, N<2-ACETYL-N-BENZYL-, ASPARAGINE, N,N<2-DIBENZYL-, ETHYL ESTER, HYDROCHLORIDE, DL-, MALAMIDE, N<1,N<4-DIBENZYL-, MALAMIDE, N<1,N<4-DIBENZYL-, ASPARTIC ACID, N-BENZYL-, DL-, 3-PYRROLIDINECARBOXYLIC ACID, 3-ACETAMIDO-1-BENZYL-2,5-DIOXO-, ETHYL ESTER	737 13216 740	15074 15074 15076	241 N 241 N 242 N	7265 7265 23008	4666 4666
SUCCINIMIDE, 2-ACETAMIDO-N-BENZYL-2-CARBOXY-, ETHYL ESTER	741 13211	15077 15077	243 NAB 243 NAB		
BENZENE, P-DIBUTOXY-, 2-BUTENOIC ACID CROTONIC ACID	743 744	160 15079	244 N 245 N	27505 7267	4668
P-BENZOQUINONE S	744	15079	245 N	7267	4668
2,5-CYCLOHEXADIENE-1,4-DIONE	748	161	246 N	708	132
P-QUINONE	749	8091	247 N	10317	133
SUCCINAMIDE, 2-/BENZYLAMINO/-N,NPR-DIBENZYL-, TOLUENE, A,A,2,3,4,5,6-HEPTACHLORO-, TOLUENE, A,2,3,4,5,6-HEXACHLORO-, BENZOIC ACID	749 751 2216 751 751 774	8091 21019 21019 21019 21019 15082	247 N 248 N 248 N 248 N 248 N 249 N	10317 10391 10391 10391 10391	133 2810 2810 2810 2810
ANILINE, 2,5-DICHLORO-, ANILINE, O-CHLORO-, BIPHENYL	774	41177P	250 N		
PHENANTHRENE	776	29322	251 N	16907	4818
GERMANE, BENZYLTRICYCLOHEXYL-, CARBOLIC ACID	779	162	252 N B	57	4671
PHENOL	780	8093	253 N	58	4672
O-CRESOL	781	8094	254 N	59	818
ACETIC ACID, BENZYL ESTER	783	163	255 N	V 289	134
NICOTINAMIDE	810	8035	256 N	61	136
ACETONITRILE, /M-METHOXYPHENYL/-, M-TOLUIDINE, A,A,A-TRIFLUORO-, P-XYLENE, A,A,A,APR,APR,APR-HEXAFLUORO-, NAPHTHALENE	821 843 844 859 860 861 863 864	41202P 165 166 167 8106 41224P 168 41226P	257 N 258 N 259 N B 260 N 261 NA 262 N 263 N 264 N	3152 3152 3153 10222 10223 1401 9542	137 137 2009 138 4440 820
BENZYLAMINE	865	169	265 N	62	139
CINNAMIC ACID, O-CHLORO-, A-TOLUENESULFONAMIDE	866	170	266 N	63	140
BENZO/DEF/PHENANTHRENE	867	171	267 N B	23009	4678
PYRENE	869	172	268 N	10195	4819
ACETOPHENONE, 4-METHYL-, BENZYLAMINE, N-METHYL-, ACENAPHTHENE	870 870 872 873	173 173 174 8107	269 N 269 N 270 N 271 N	64 64 10188 3731	141 141 435 142
ACENAPHTHENE	875	548	272 N	65	143
ACENAPHTHENE	875	175	272 N	65	143
ACENAPHTHENE	7458	175	272 N	65	143
ACENAPHTHENE	7458	548	272 N	65	143
ACENAPHTHYLENE, 1,2-DIHYDRO-, ACENAPHTHYLENE, 1,2-DIHYDRO-, ACENAPHTHYLENE, 1,2-DIHYDRO-, ACENAPHTHYLENE, 1,2-DIHYDRO-, MALEIC ACID, DIBUTYL ESTER	875 875 7458 7458 878	175 548 175 548 176	272 N 272 N 272 N 272 N 273 N	65 65 65 65 680	143 143 143 143 144
3-PENTANONE	880	28516	274 N	10224	436
ACETIC ACID, PHENYL-, ETHYL ESTER	882	10770	275 N	J 110	437
CINNAMIC ACID, ETHYL ESTER	884	177	276 N	718	147
BENZENEDIAZONIUM CHLORIDE, P-/DIETHYLAMINO/-, CMPD WITH ZINC CHLORIDE	888	41231P	277 N	19833	3802
BENZENEDIAZONIUM CHLORIDE, P-/DIETHYLAMINO/-, CMPD WITH ZINC CHLORIDE	889	41232P	277 N	19833	3802
BENZENEDIAZONIUM TRICHLOROZINCATE, P-/DIETHYLAMINO/-, BENZENEDIAZONIUM TRICHLOROZINCATE, P-/DIETHYLAMINO/-, BENZYL ALCOHOL, N-METHYL-, P-XYLENE, A-CHLORO-, ANTHRANILIC ACID, METHYL ESTER	888 889 889 894 895 897	41231P 41232P 41232P 28517 178 28519	277 N 277 N 277 N 278 NA 279 N 280 NAB	19833 19833 19833 67 68 1200	3802 3802 3802
BENZ/A/ACENAPHTHYLENE	901	180	281 N	6679	151
FLUORANTHENE	901	180	281 N	6679	151
FUMARIC ACID, DIETHYL ESTER	908	28520	282 N	V 213	154
ANTHRANILIC ACID, BUTYL ESTER	91	182	283 NA	655	155
ETHER, ETHYL 2-NAPHTHYL, NAPHTHALENE, 2-ETHOXY-,	918 918	29698 29698	284 N 284 N	72 72	4679 4679

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BENZOIC ACID, P-TOLYL ESTER	921	185	285 N B	1187	157
P-CRESOL, BENZOATE	921	185	285 N B	1187	157
BENZIL	922	186	286 N	73	158
BIBENZOYL	922	186	286 N	73	158
GLYOXAL, DIPHENYL-	922	186	286 N	73	158
PROPIONIC ACID, BENZYL ESTER	929	187	287 N	311	441
BUTYRIC ACID, BENZYL ESTER	930	188	288 N	726	442
ACETIC ACID, PHENYL-, PENTYL ESTER	938	15097	289 N		
2-INDOLINE, 3,3-BIS/P-HYDROXY-PHENYL/-, DIACETATE	939	29137	290 NAB	3980	
ISACEN	939	29137	290 NAB	3980	
OXINDOLE, 3,3-BIS/P-HYDROXY-PHENYL/-, DIACETATE	939	29137	290 NAB	3980	
PROPANE, 1-CHLORO-1-NITRO-,	943	189	291 N	10181	159
ETHANE, 1-CHLORO-1-NITRO-,	944	190	292 N	9145	443
PROPANE, 1,1-DICHLORO-1-NITRO-,	945	191	293 N	10182	444
PROPANE, 2-CHLORO-2-NITRO-,	946	192	294 N	6339	160
ANTHRANILIC ACID, ISOBUTYL ESTER	949	193	295 N	10191	1839
BENZYL ALCOHOL, O-CHLORO-A-METHYL-,	1595	8179	296 N	18673	
PHTHALIC ACID, DIMETHYL ESTER	969	197	297 N	10384	
SEBACIC ACID, BENZYL OCTYL ESTER	974	15100	298 N	6557	162
PHENOL, 2,4-BIS/1-METHYLBUTYL/-,	984	198	299 N		
MALEIC ACID, DIMETHYL ESTER	986	28521	300 N	723	164
1,6-NAPHTHALEDIOL	994	15293	301 N	6943	3602
SEBACIC ACID, BENZYL BUTYL ESTER	1000	15103	302 N	6558	1843
BENZENE, O-DICHLORO-,	1003	201	303 N	746	1844
BENZOIC ACID, ISOBUTYL ESTER	1006	202	304 N	75	1845
SALICYLIC ACID, ISOBUTYL ESTER	1007	203	305 N	724	1846
MENTHOL, SALICYLATE	1008	204	306 N	9725	
SALICYLIC ACID, P-MENTH-3-YL ESTER	1008	204	306 N	9725	
AZOLE	1010	29556	307 N	10330	166
PYRROLE	1010	29556	307 N	10330	166
1H-PYRROLE	1010	29556	307 N	10330	166
INDENE	1012	10938	308 N	V 227	446
BENZOPHENONE, 4,4*-DICHLORO-,	1014	206	309 N	10392	
PHENOL, 2-TERT-BUTYL-6-ISOPROPYL-,	1016	15105	310 N	6615	2010
ISOEUGENOL, TRANS-,	1017	8115	311 N	76	2011
PHENOL, 2-METHOXY-4-PROPENYL-,	1017	8115	311 N	76	2011
TRANS-,					
METHANE, DIPHENYL/O-NITROPHENYL/-,	1022	41281P	312 N		
TOLUENE, A,A-DIPHENYL-O-NITRO-,	1022	41281P	312 N		
ETHER, METHYL 2-NAPHTHYL,	1026	15296	313 N	77	6405
NAPHTHALENE, 2-METHOXY-,	1026	15296	313 N	77	6405
FORMANILIDE	1031	29699	314 NA	25009	6001
CAFFEINE	1036	209	315 N	10393	
XANTHINE, 1,3,7-TRIMETHYL-,	1036	209	315 N	10393	
BENZENE, 1,2,4-TRIMETHYL-,	1038	8116	316 N	3417	170
PSEUDOCUMENE	1038	8116	316 N	3417	170
M-XYLENE	1045	210	317 N	10394	171
BENZALDEHYDE, 3-ETHOXY-4-HYDROXY-,	1051	211	318 N	1320	
BENZALDEHYDE, 3-ETHOXY-4-HYDROXY-,	5178	211	318 N	1320	
BENZALDEHYDE, 3-ETHOXY-4-HYDROXY-,	8655	211	318 N	1320	
BOURBONAL	1051	211	318 N	1320	
BOURBONAL	5178	211	318 N	1320	
BOURBONAL	8655	211	318 N	1320	
VANILLIN, ETHYL-,	1051	211	318 N	1320	
VANILLIN, ETHYL-,	5178	211	318 N	1320	
VANILLIN, ETHYL-,	8655	211	318 N	1320	
BENZOIC ACID, METHYL ESTER	1052	212	319 N	78	172
1-BENZAZINE	1053	213	320 N	6683	4683
QUINOLINE	1053	213	320 N	6683	4683
QUINALDINE	1055	15107	321 N	6393	2811
QUINOLINE, 2-METHYL-,	1055	15107	321 N	6393	2811
O-CRESOL, 4-TERT-BUTYL-,	1061	8118	322 N B	527	
PHENOL, 2,5-DIMETHYL-,	1065	10846	323 N B	82	6406
2,5-XYLENOL	1065	10846	323 N B	82	6406
2,5-XYLENOL S	1169	10846	323 N B	82	6406
BENZENE, 1-ISOPROPYL-4-METHYL-,	1066	15109	324 N	V 268	447
P-CYME	1066	15109	324 N	V 268	447
TOLUENE, P-ISOPROPYL-,	1066	15109	324 N	V 268	447
PHENOL, 4,4*-ISOPROPYLIDENEDI-,	1070	216	325 N B	18669	176
P-CUMENOL	1073	15303	326 N	6685	177
PHENOL, P-ISOPROPYL-,	1073	15303	326 N	6685	177
1-CYCLOHEXENE-1-CARBOXANILIDE, 4-ISOPROPYL-,	1084	41300P	327 N		
PHELLANDRANILIDE	1084	41300P	327 N		
BENZENE, 1,3,5-TRINITRO-,	1086	29139	328 N	23011	6407
SEBACIC ACID, DIBENZYL ESTER	1106	18407	329 N	7638	180
4-BIPHENYLOL	1107	21023	330 NAB	10383	6202
PHENOL, P-PHENYL-,	1107	21023	330 NAB	10383	6202
BENZOIC ACID, 2,4,6-TRINITRO-,	1112	217	331 N B	25010	
BENZYL ALCOHOL, A-METHYL-, ACETATE	1114	8126	332 N	312	181
COUMARIN, 5,7-DIHYDROXY-3,4-DIMETHYL-,	1116	15305	333 NAB		

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BENZOIC ACID, 2,4,6-TRIHYDROXY-,	1122	15306	334 NAB	27509	
BENZ/A/ANTHRACENE	1124	15114	335 N	6018	6203
BENZ/A/ANTHRACENE	9258	15114	335 N	6018	6203
AZOXYBENZENE	1132	15308	336 N	10412	4210
AZOXYBENZENE	5184	15308	336 N	10412	4210
AZOXYBENZENE	11984	15308	336 N	10412	4210
PIPERIDINIUM IODIDE, 1-METHYL-1-	1134	41318P	337 N		
/2-/9-PHENYL-9-THIOXANTHYLOXY/ETHYL/-,					
AMMONIUM IODIDE, DIETHYLMETHYL-2-	1135	41319P	338 N		
/9-PHENYL-9-THIOXANTHYLOXY/ETHYL/-,					
EREMORPHILONE, HYDROXY-, BENZOATE	1137	41320P	339 N		
NAPHTHALENE, 2/3H/-, 4,4A,5,6,7-	1137	41320P	339 N		
8-HEXAHYDRO-1-HYDROXY-3-ISOPROPYLIDENE-					
4A,5-DIMETHYL-, BENZOATE	1145	219	340 N	6527	
NAPHTHALENE, 2,3-DIMETHYL-,	8569	219	340 N	6527	
NAPHTHALENE, 2,3-DIMETHYL-,	1146	15309	341 NAB	6528	6408
2-BIPHENYLOL	1146	15309	341 NAB	6528	6408
PHENOL, O-PHENYL-,	1192	15309	341 NAB	6528	6408
PHENOL, O-PHENYL-, K	1153	32505	342 N	81	6410
ACRIDINE	1153	32505	342 N	81	6410
10-AZAANTHRACENE	1154	15118	343 NAB	6529	6411
BIPHENYLDIOL, 2,2*-,	1154	15118	343 NAB	6529	6411
PHENOL, 2,2PR-DI-,	1155	15310	344 NAB		
TOLUENE-2,4,6-TRIAMINE	1157	29140	345 N		
FUMARAMIDE, N,NPR-DIISOPROPYL-,	1171	28007	346 N	9440	
INDOLE, 2-METHYL-,	1175	41337P	347 N		
CINNAMIC ACID, 3,4-METHYLENEDIOXY-,					
ETHYL ESTER	1177	220	348 N B	656	
CINNAMIC ACID, 4-HYDROXY-3-					
METHOXY-, ETHYL ESTER	1177	220	348 N B	656	
FERULIC ACID, ETHYL ESTER	1183	15646	349 N	83	1408
PHENOL, 3,5-DIMETHYL-,	8080	15646	349 N	83	1408
PHENOL, 3,5-DIMETHYL-,	1183	15646	349 N	83	1408
3,5-XYLENOL	8080	15646	349 N	83	1408
3,5-XYLENOL	1185	41344P	350 N		
FUMARAMIDE, N,NPR-DICYCLOHEXYL-,	1188	221	351 N	31624	
CHRYSENE	7539	221	351 N	31624	
CHRYSENE	1190	222	352 N	1201	187
NAPHTHALENE, 2,6-DIMETHYL-,	1191	223	353 N	25011	
11H-BENZO/B/FLUORENE	1198	8129	354 NAB		
THIAZOLE, 2,4-DIAMINO-,					
HYDROCHLORIDE	13386	224	355 N	85	
BENZENE, 1,2,4,5-TETRAMETHYL-,	1199	224	355 N	85	188
BENZENE, 1,2,4,5-TETRAMETHYL-,	1199	224	355 N	85	188
DURENE	13386	224	355 N	85	
DURENE	1202	41349P	356 N		
PENTANOIC ACID, 3-BENZAMIDO-					
3-ETHYL	1202	41349P	356 N		
VALERIC ACID, 3-BENZAMIDO-3-ETHYL-,	1207	41352P	357 N		
2-PROPANONE, /4-HYDROXY-3-METHOXY-					
PHENYL/-,	1208	8130	358 N		
5H-DIINDENO/1,2-A 1PR,2PR-C/FLUORENE,					
10,15-DIHYDRO-,	1208	8130	358 N		
TRIBENZYLENEBENZENE	1208	8130	358 N		
TRUXENE	1210	41353P	359 N		
BUTYRIC ACID, 3-BENZAMIDO-2-					
ISOPROPYL-3-METHYL-,	1211	36762	360 N		
NAPHTHACENE	1212	41354P	361 N		
BUTYRIC ACID, 3-BENZAMIDO-2-ISO-					
PROPYL-3-METHYL-, ETHYL ESTER	1215	36011	362 N		
PHENOL, P-NONYL-, /MIXTURE OF					
ISOMERS/	1218	41357P	363 N		
CYCLOPENTANEACETIC ACID, 1-					
BENZAMIDO-,	1220	41359P	364 N		
HYDRATROPIC ACID, A-BENZAMIDO-,	1221	41360P	365 N		
CAPRYLIC ACID, B-METHYL-B-					
/P-METHYLBENZAMIDO/-,	1221	41360P	365 N		
OCTANOIC ACID, 3-METHYL-3-					
/P-METHYLBENZAMIDO/-,	1222	28529	366 N		
BUTYRIC ACID, 3-BENZAMIDO-3-METHYL-					
2-PHENYL-,	1230	36013	367 N		
M-CRESOL, 4,5-DIAMYL-,	1230	36013	367 N		
M-CRESOL, 4,5-DIPENTYL-,	1231	15121	368 N	6616	2817
P-CRESOL, 2-/A-METHYLBENZYL/-,	1232	41363P	369 N		
M-CRESOL, 6-AMYL-,	1234	8131	370 N B	673	1409
O-CRESOL, 6-TERT-BUTYL-,	1245	28530	371 N	1202	6205
2*-ACETONAPHTHONE	1250	15123	372 N	6074	4445
PYRIDINE, 3-ETHYL-,	1253	15315	373 N	86	
BIPHENYL, 2-NITRO-,	1259	8134	374 N		
ALLOISOLEUCINE, DL-,	1259	18606	374 N		
ALLOISOLEUCINE, DL-,	1259	18606	374 N		
VALERIC ACID, 2-AMINO-3-METHYL-,					
VALERIC ACID, 2-AMINO-3-METHYL-,	1259	8134	374 N		

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COUMARIN, 3-METHYL-,	1260	28532	375 N	87	6415
ANILINE, M-CHLORO-,	1262	28533	376 N	88	190
ETHANE, 1,1-DICHLORO-1-NITRO-,	1263	226	377 N	10364	2820
PHTHALIC ACID, DIMETHYL ESTER	1265	8135	378 N	89	191
M-CRESOL, 4,6-DI-TERT-BUTYL-,	262	4896	379 N	10197	
BENZOTRICHLORIDE	1268	227	380 N	90	193
TOLUENE, A,A,A-TRICHLORO-,	1268	227	380 N	90	193
GLYCINE, N-/N-CARBOXYSELYL/-,	1269	8137	381 N	2823	
N-BENZYL ETHYL ESTER, DL-,					
PHTHALIC ANHYDRIDE, TETRACHLORO-,	1271	228	382 N		
M-ANISALDEHYDE, 2-HYDROXY-,	1273	8138	383 NAB	528	6803
M-ANISALDEHYDE, 2-HYDROXY-,	1273	9997	383 NAB	528	6803
BENZALDEHYDE, 2-HYDROXY-3-METHOXY-,	1273	9997	383 NAB	528	6803
BENZALDEHYDE, 2-HYDROXY-3-METHOXY-,	1273	8138	383 NAB	528	6803
O-VANILLIN	1273	8138	383 NAB	528	6803
O-VANILLIN	1273	9997	383 NAB	528	6803
2-BIPHENYLAMINE	1275	28230	384 N	9421	6416
ANILINE, O-NITRO-,	1276	229	385 N	6495	454
PHENOL, O-/A-METHYLBENZYL/-,	1286	15126	386 N	6617	4019
ANILINE, 2,4-DINITRO-,	1287	231	387 N	3290	4211
DIPHENYLAMINE, 2-NITRO-,	1292	232	388 N	681	1483
DIPHENYLAMINE, 2-NITRO-,	8351	232	388 N	681	1483
BENZALDEHYDE, 2,3-DIMETHOXY-,	1294	33344	389 N	10405	
O-VERATRALDEHYDE	1294	33344	389 N	10405	
BENZOTHAZOLE, 2-MERCAPTO-,	1298	8139	390 N	10149	6602
BENZOTHAZOLE, 2-MERCAPTO-,	11493	8139	390 N	10149	6602
2-BENZOTHAZOLETHIOL	1298	8139	390 N	10149	6602
PHTHALIC ACID, DIPHENYL ESTER	1304	235	391 N	93	197
P-ANISIDINE	1305	28232	392 N	94	198
ANILINE, P-CHLORO-,	1317	8140	393 N	10490	200
ANTHRACENE	1319	239	394 N	25016	
ACETIC ACID, 2,4,5-TRICHLORO-	1323	28234	395 N	10406	6419
PHENOXY-, ISOPROPYL ESTER					
GUANIDINE, 1,3-DIPHENYL-,	1337	8143	396 N	97	6421
TYROSINE, N-CARBOXY-, N-BENZYL	1338	8144	397 N		
ESTER, BENZYL CARBONATE, L-,					
NAPHTHO/2,3-D/-1,3-DIOXOLE-6-	1342	15130	398 N	6946	
CARBOXYLIC ACID, 8-HYDROXY-7-/HYDROXY-					
METHYL/-5,6,7,8-TETRAHYDRO-5-/3,4,5-					
TRIMETHOXYPHENYL/-, G-LACTONE /ISOMER/					
PICROPDOPHYLLIN, /PLUS/-,	1342	15130	398 N	6946	
1,3-PROPANEDIOL, 2-HYDROXYMETHYL-	1346	242	399 N	1203	203
2-NITRO-,					
PHENOL, 4,4PR-SULFONYLDI-,	1352	15321	400 N	6020	826
NICOTINE	1355	8148	401 N	V 269	1207
PYRROLIDINE, 1-METHYL-2-/3-PYRI-	1355	8148	401 N	V 269	1207
DYL/-,					
GLYCINE, N-/N-CARBOXYVALYL/-,	1370	8150	402 N		
N-BENZYL ESTER, DL-,					
PYRIDINIUM CHLORIDE, 1-DODECYL-,	1373	28237	403 N	10396	2012
O-CRESOL, 4-CHLORO-A-PHENYL-,	1374	15322	404 N	6919	2827
BENZENESULFONYL FLUORIDE,	1380	15325	405 N	7052	208
P-CHLORO-,					
ISOPSEUDOCUMENOL	1382	18410	406 N	8659	6208
PHENOL, 2,3,5-TRIMETHYL-,	1382	18410	406 N	8659	6208
HYDRACRYLIC ACID, 3,3-BIS/P-CHLORO-	1389	41415P	407 N		
PHENYL/-, METHYL ESTER					
BENZOIC ACID, COPPER /II/ SALT	1415	41436P	408 N		
COPPER /II/ BENZOATE	1415	41436P	408 N		
PHENOL, P-CHLORO-,	1418	243	409 N	17044	210
2-FUROIC ACID, 5-NITRO-,	1424	244	410 N B	10354	
2-FURANMETHANEDIOL, 5-NITRO-, DI-	1428	18016	411 NAB	8614	
ACETATE					
2-FUROIC ACID, 5-NITRO-, ETHYL ESTER	1434	245	412 N B	691	6209
2-FURALDEHYDE, 5-NITRO-,	1435	36513	413 N	23016	
2-FUROIC ACID, 5-NITRO-, METHYL ESTER	1436	41445P	414 N		
BARIUM BENZOATE, DIHYDRATE	1437	15330	415 N	6333	
BENZOIC ACID, BARIUM SALT,	1437	15330	415 N	6333	
DIHYDRATE					
1-NAPHTHALENEETHANOL, 2-HYDROXY-	1453	41459P	416 N		
B-PHENYL-,					
ACETIC ACID, /2-NAPHTHYLOXY/-	1455	41461P	417 N		
PHENYL-,					
2-BUTENAL	1457	29705	418 N	V 60	
CROTONALDEHYDE	1457	29705	418 N	V 60	
ANETHOL	1467	8156	419 N	V 258	213
ANISOLE, P-PROPENYL-,	1467	8156	419 N	V 258	213
ACETIC ACID; FURFURYL ESTER	1475	249	420 NAB	10445	459
FURFURYL ALCOHOL, ACETATE	1475	249	420 NAB	10445	459
FURFURYL ALCOHOL, 5-NITRO-, ACETATE	1476	41467P	421 NAB		
M-XYLENE, 5-TERT-BUTYL-2,4,6-TRI-	1479	250	422 N	6497	4212
NITRO-,					
PHENOL, P-METHOXY-,	470	10768	423 N	3154	97

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PHENOL, P-METHOXY-,	1482	10768	423 N	3154	
CINNAMALDEHYDE	1490	18891	424 N	101	216
SALICYLIC ACID, P-AMINO-, SODIUM SALT	1494	15333	425 NAB	6187	
BENZOIC ACID, ETHYL ESTER	1506	252	426 N	1204	219
BENZOIC ACID, BENZYL ESTER	1509	253	427 N	V 627	2833
CARBANILIC ACID, FURFURYL ESTER	1514	41481P	428 N		
FURFURYL ALCOHOL, CARBANILATE	1514	41481P	428 N		
1,5-NAPHTHALENEDIOL	1519	15141	429 N	7290	6603
CINNAMIC ACID, BENZYL ESTER	1520	21026	430 N	104	6428
ACETIC ACID, CINNAMYL ESTER	1521	254	431 N	682	222
SALICYLIC ACID, ISOPENTYL ESTER	1522	255	432 N B	1189	1208
SALICYLIC ACID, BENZYL ESTER	1523	256	433 N B	719	1411
ANTHRANILIC ACID, N-METHYL-, METHYL ESTER	1527	32008	434 N	9423	2835
STYRENE, 8-BROMO-,	1529	8158	435 N	V 497	221
FORMIC ACID, BENZYL ESTER	1531	15143	436 N	6694	
PHTHALIDE, 3,3-BIS/5-HYDROXYCAR-VACRYL/-,	1532	8159	437 N B	10802	
THYMOLPHTHALEIN	1532	8159	437 N B	10802	
ANISOLE, 2-BENZYLOXY-5-PROPENYL-,	1533	15335	438 N	6695	2836
BENZENE, 1-BENZYLOXY-2-METHOXY-4-PROPENYL-,	1533	15335	438 N	6695	2836
BENZYL ISOEUGENOL	1533	15335	438 N	6695	2836
2-NAPHTHALENESULFONIC ACID, 6,7-DIHYDROXY-, SODIUM SALT	1536	18017	439 N	27514	
2-NAPHTHALENESULFONIC ACID, 6,7-DI-HYDROXY-, SODIUM SALT K	9550	18017	439 N	27514	
2-FURALDEHYDE, 5-NITRO-, SEMICARB-AZONE	1538	15144	440 NAB	6416	
BENZOIC ACID, P-AMINO-,	1542	15145	441 N	6944	6429
O-TOLUIDINE	1543	8160	442 N	107	225
M-TOLUIDINE	1544	8161	443 NA	108	226
ABIETIC ACID, DEHYDRO-,	1545	29146	444 N	25019	
1-PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-ISOPROPYL-,	1545	29146	444 N	25019	
GLUTARIC ACID, 3-/P-METHOXY-PHENYL/-,	1549	41487P	445 N	27515	
GLUTARIC ACID, 3-/3-BENZYLOXY-4-METHOXYPHENYL/-,	1550	15146	446 N	10849	
GLUTARIC ACID, 3-/3-ETHOXY-4-METHOXYPHENYL/-,	1562	29147	447 N	25020	
2-PROPANOL, 1-/O-TOLUIDINO/-,	1566	15147	448 N	10515	
ANILINE, O-MERCAPTO-,	1568	15148	449 N	8764	6431
BENZENETHIOL, O-AMINO-,	1568	15148	449 N	8764	6431
ACETIC ACID, /3,4-DICHLORO-PHENOXY/-,	1571	33345	450 N	4276	6432
ACETIC ACID, /3,4-DICHLORO-PHENOXY/-,	13144	33345	450 N	4276	6432
P-TOLUENESULFONIC ACID, METHYL ESTER	1572	18411	451 N	6696	227
2-FURANMETHANEDIOL, DIBUTYRATE	1573	41495P	452 N		
PHENOL, 2-2*-METHYLENEBIS/3,4,6-TRICHLORO-,	1576	15150	453 NAB	7839	6434
DIBENZYLAMINE, N-/2-CHLOROETHYL/-,	1577	41496P	454 N		
BENZENE, 1-ETHYL-2-NITRO-,	1579	28240	455 N	109	228
ACETIC ACID, /2,5-DICHLORO-PHENOXY/-,	1584	41499P	456 NAB		
ACETIC ACID, /2,5-DICHLORO-PHENOXY/-,	13142	47358P	456 NAB		
ACETIC ACID, /P-CHLOROPHENOXY/-,	1590	259	457 N	10777	6436
ACETIC ACID, /P-CHLOROPHENOXY/-,	13139	259	457 N	10777	6436
FUMARIC ACID, DIMETHYL ESTER	1600	260	458 N	110	229
ISOTHIOCYANIC ACID, ALLYL ESTER	1603	8182	459 N B	3155	2839
ANILINE, O-AMINO-,	1604	262	460 NA	112	231
1,2-BENZENEDIAMINE	1604	262	460 NA	112	231
O-PHENYLENEDIAMINE	1604	262	460 NA	112	231
ETHANOL, 2,2*-/M-TOLYLIMINO/DI-,	1614	28511	461 N	10415	4817
ETHANOL, 2,2PR-/M-TOLYLIMINO/DI-,	752	28511	461 N	10415	4817
BENZOIC ACID, P-ETHOXY-,	1623	15151	462 N B	6972	6439
BENZOIC ACID, P-ETHOXY-, /KBR/	11182	15151	462 N B	6972	6439
KETONE, PHENYL 2-THIENYL,	1627	9998	463 N	6920	6441
PYRIDINIUM HYDROXIDE, 1-/2-ETHOXY-1-ETHOXYCARBONYL-2-HYDROXY/VINYL/-, INNER SALT	1629	41521P	464 NAB		
1H-BENZOTRIAZOLE	1631	15152	465 N	6410	828
1H-BENZOTRIAZOLE	10542	15152	465 N	6410	828
PHENETHYL ALCOHOL	1632	8184	466 N	113	
ACETIC ACID, PHENYL-, PHENETHYL ESTER	1633	265	467 N	720	829
BUTYRIC ACID, PHENETHYL ESTER	1648	266	468 N	727	461
ACETIC ACID, 3-PHENYLPROPYL ESTER	3862	15338	469 N	6697	236
ACETIC ACID, PHENYL-, PHENETHYL ESTER	1650	15338	469 N	6697	236