HANDBOOK of

DATA ON COMMON ORGANIC COMPOUNDS

VOLUME III

CAS Registry Number Index
Molecular Formula Index
Name/Synonym Index

Editors

David R. Lide
G.W.A. Milne

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CRC Press
Boca Raton Ann Arbor London Tokyo

Library of Congress Cataloging-in-Publication Data

Handbook of data on common organic compounds / edited by David R. Lide and G.W.A. Milne.
p. cm.
Includes indexes.
Contents: v. 1. Compounds A—E -- v. 2. Compounds F—Z -- v. 3. Indexes.
ISBN 0-8493-0404-0 (set : alk. paper)
1. Organic compounds--Tables. I. Lide, David R., 1928— . II. Milne, George W.A., 1937—
QD257.7.H35 1995
547'.00212--dc20 94-39019
CIP

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Mass spectra with the mass spectra reference identified as NIST were obtained from the NIST/EPA/MSDC Mass Spectral Database, 1990 Version.

The relative intensities of the Mass spectral peaks from the NIST/EPA/MSDC Mass Spectral Database were modified from a scale of 1000 to a scale of 100 for use in Data on Common Organic Compounds.

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No claim to original U.S. Government works
International Standard Book Number 0-8493-0404-0
Library of Congress Card Number 94-39019
Printed in the United States of America 2 3 4 5 6 7 8 9 0
Printed on acid-free paper

THE EDITORS

David R. Lide has been Editor-in-Chief of the *CRC Handbook of Chemistry and Physics* since 1989. He received his B.S. in Chemistry from Carnegie Institute of Technology in 1949, M.A. in Physics from Harvard in 1951, and Ph.D. in Chemical Physics from Harvard in 1952. He was a staff member of the National Bureau of Standards (now the National Institute of Standards and Technology) from 1955 to 1988, where he carried out research in microwave and infrared spectroscopy, molecular structure, high temperature chemistry, and infrared lasers. In 1969 he became Director of the Standard Reference Data Program at NBS, a national effort to produce critically evaluated databases of physical, chemical, and materials properties. He founded the *Journal of Physical and Chemical Reference Data*, published jointly by NBS, the American Chemical Society, and the American Institute of Physics, and served as Editor from 1972 to 1992. He has served as President of the Committee on Data for Science and Technology (CODATA) of the International Council of Scientific Unions, President of the Physical Chemistry Division of the International Union of Pure and Applied Chemistry (IUPAC), Chairman of the IUPAC Committee on Chemical Databases, Chairman of the American Chemical Society Task Force on Scientific Numerical Databases, and Councilor of the American Physical Society. Membership on advisory boards includes Chemical Abstracts Service, Petroleum Research Fund, Engineering Information, Inc., National Materials Property Data Network, Chemistry Departments at Harvard and Princeton, and various panels of the National Academy of Sciences. He held a Fulbright Fellowship at Oxford in 1952-53 and National Science Foundation Senior Postdoctoral Fellowships at University College London in 1959-60 and the University of Bologna in 1968-69. Awards include the Department of Commerce Gold Medal in 1969, the Samuel Wesley Stratton Award in 1969, a Presidential Rank Award of Meritorious Federal Executive in 1986, the Herman Skolnik Award in Chemical Information in 1988, and the Patterson-Crane Award of the American Chemical Society in 1991. He is the author of two books, *Basic Laboratory and Industrial Chemicals* and *Handbook of Thermophysical and Thermochemical Data*, as well as more than 100 research papers.

George W.A. Milne is a Research Chemist in the National Cancer Institute, one of the National Institutes of Health in Bethesda, MD. He obtained his B.Sc. (1957), M.Sc. (1958), and Ph.D. (1960) degrees from the University of Manchester in England and spent two postdoctoral years at the University of Wisconsin before joining NIH in 1962. His research interests have included organic and natural products chemistry and analytical chemistry, and he spent over ten years working on the application of mass spectrometry to identification of organic compounds. This work led to the development in 1972 of the NIH/EPA Mass Spectral Database, which was the first computer-searchable mass spectral library. Since the mid-seventies, Dr. Milne has worked increasingly in the application of computers in chemistry and currently heads a group which is using molecular modeling in design of drugs for the treatment of cancer and AIDS. He has published over 150 papers and one book and since 1989 has been Editor-in-Chief of the American Chemical Society's *Journal of Chemical Information and Computer Sciences.*

INTRODUCTION

The information on each compound in the *Handbook of Data on Common Organic Compounds*, is presented in a standard format which is described below. Compounds are listed in approximate, but not exact, alphabetical order by principal name; certain deviations from a strict systematic order were necessary to achieve the most efficient page layout. The most effective way to locate a compound is to use the Name/Synonym Index, which includes the principal name and an average of four synonyms per compound. Indexes to molecular formula and CAS Registry Number are also provided. The indexes give the sequential identification number assigned to each compound.

The data presented in this work have been taken from many sources, both compilations and original literature. Space considerations preclude giving specific references to the sources of physical property data, but some of the most useful general sources are listed at the end of this Introduction. Sources of spectral data are referenced by codes which are explained in the List of Abbreviations. The explanation of the data fields follows.

Data Fields and Explanations

Name: Generally, the Index Name from the *8th* or *9th Collective Index* of Chemical Abstracts Service (CAS).[1] In some cases, especially pesticides and pharmaceuticals, the common name is used rather than the more complex CAS systematic name.

Synonym: A synonym in common use. When the primary name is non-systematic, the systematic name appears here.

LF: In many cases the line formula, a linear array of the atoms or groups in the sequence in which they appear in the molecule, is given.

MF: The molecular formula written in the Hill Order.[1]

CAS RN: The Chemical Abstracts Registry Number assigned by CAS as a unique identifier for the compound.

Beil RN: The Beilstein Registry Number used as a unique identifier in the *Beilstein Database*.[2]

Beil Ref: Citation to the printed *Beilstein Handbook of Organic Chemistry*.[3] An entry of 5-18-11-01234, for example, indicates that the compound may be found in the 5th Series, Volume 18, Subvolume 11, page 1234.

Merck No: Monograph Number in *The Merck Index, Eleventh Edition*.[4] It should be noted that this is not a unique identifier for a single compound, since several derivatives or isomers of a compound may be included in the same Monograph.

MW: Molecular weight (relative molar mass) as calculated with the 1991 IUPAC Standard Atomic Weights.[5]

MP: Normal melting point in °C. Although some values are quoted to 0.1°C, uncertainties are typically several degrees Celsius. A value is sometimes followed by "dec", indicating decomposition is observed at the stated temperature (so that it is probably not a true melting point). See the List of Abbreviations for other abbreviations.

BP: Boiling point in °C. When available, the normal boiling point is given first, without a superscript. This is the temperature at which the liquid phase is in equilibrium with the vapor at a pressure of 760 mmHg (101.325 kPa). Boiling point values at reduced pressure are also given in many cases; here the superscript indicates the pressure in mmHg. A "dec" or "exp" following the value indicates decomposition or explosion has been observed at the boiling point. A simple entry of "exp" (sometimes followed by a temperature) indicates explosion may occur on heating, even below the boiling point. An entry of "sub" indicates that no boiling point is available, but measurable vapor (sublimation) pressure has been observed upon heating the solid. A temperature may be given, but no precise meaning can be attached because the pressure is not specified.

VP: Vapor pressure in kPa at the temperature indicated by the superscript (in °C). Note that 1 kPa = 7.50 mmHg and 101.325 kPa = 1 atmos.

Density: Mass per unit volume in g/cm^3. The superscript indicates the temperature. Values are given only for the liquid and solid phases, and all values are true densities, not specific gravities. The number of decimal places gives a rough estimate of the accuracy of the value.

n: Refractive index, at the temperature indicated by the superscript. All values refer to a wavelength of 589 nm (sodium D line). Values are given only for liquids and solids.

[α]: Specific rotation in degrees. This is the angle by which the plane of polarization of an incident light beam is rotated while traversing a 1 dm path, for the concentration and solvent indicated. A measurement made at a wavelength of 5893 (the sodium D line) is indicated by a superscript such as 25/D, where 25 is the temperature in °C . When a different wavelength was used, the wavelength value in Å is given as a subscript.

Color: The color, crystalline form, and solvent from which the compound was crystallized are given in abbreviated form (see List of Abbreviations).

Sol: Solubility on a relative scale: 1 = insoluble; 2 = slightly soluble; 3 = soluble; 4 = very soluble; 5 = miscible; 6 = decomposes. See List of Abbreviations for the solvent abbreviations.

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Spectral Data

Mass, Infrared, Ultraviolet, Raman, and Nuclear Magnetic Resonance (including Proton and Carbon-13) spectral data are given when available. For each, the reference code is cited first in bold type; peak information follows. See the List of Abbreviations for the meaning of the reference codes.

MS: The m/e values of the most abundant peaks are shown. The relative intensities are given in parentheses, with the strongest peak assigned an intensity of (100).

IR: Major infrared peaks in cm^{-1}. All absorption bands characteristic of a functional group were coded. In addition, at least one strong band in each micrometer or 100 cm^{-1} interval , from 3800 to 250· cm^{-1}, was coded. Spectra were coded in either micrometers or wavenumbers, depending on the format of the reference curve. Data in micrometers were converted by computer to wavenumbers for listing in the database. A micron symbol, m, is shown before the spectrum reference number for every converted spectrum. Peak positions were read to ±0.1 μm or ±10 cm^{-1}.

UV: All major ultraviolet bands, their molar absorption coefficients (in parentheses, when given), and the solvent used were coded. The wavelength range was from 170 to 600 nm, and peaks were read to ±1 nm. When the spectrum showed vibrational fine structure, only the peak centers characteristic of the electronic transitions were recorded.

Raman: The Raman Spectra from the early API collection (#1-500) and those from *Analytical Chemistry (AC)* reference article were obtained with a mercury arc source. Only the ten strongest peaks in each spectrum were coded. Spectra were only recorded from 1700 to 150 cm^{-1} in *AC*; this is indicated by an asterisk before the first coded band. All other Raman spectra were generated using a laser source over the range 4000 to 50 cm^{-1}. In the Sadtler spectra only the parallel polarized curve was coded.

^{1}H NMR: The proton chemical shifts (δ), in ppm, for specific protons or recognizable groups, were coded to ± 0.1 ppm over the range 0 to 15 ppm, referenced to tetramethylsilane (TMS). When complex spectra due to second order effects or overlapping resonances were encountered, the range was recorded. The solvent in which the spectrum was obtained was also coded, if known.

^{13}C NMR: The carbon chemical shifts (δ), in ppm, for specific carbons or recognizable groups, were coded to ± 0.1 ppm over the range 0 to 200 ppm, referenced to tetramethylsilane (TMS). The solvent in which the spectrum was obtained was stated, if known.

Other

TLV/TWA: The threshold limit value, expressed as a time weighted average airborne concentration over a normal 8-hr workday and 40-hr workweek, to which most workers can be exposed without adverse effects. The values given here are the recommendations of the American Conference of Governmental Industrial Hygienists (ACGIH), based in part on regulations issued by the Occupational Safety and Health Administration (OSHA). Values conform to the 1992-1993 adoptions of ACGIH.[6]

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1. *Chemical Abstracts Index Guide*, Chemical Abstracts Service, Columbus, OH.
2. *The Beilstein Database*, Beilstein Institute, Frankfurt.
3. Luckenbach, R., Editor, *Beilstein Handbook of Organic Chemistry*, Springer-Verlag, Heidelberg.
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5. Lide, D.R., Editor, *CRC Handbook of Chemistry and Physics, 75th Edition*, CRC Press, Inc., Boca Raton, FL, 1994.
6. *Threshold Limit Values for Chemical Substances and Physical Agents 1992-93*, American Conference of Governmental Industrial Hygienists, Cincinnati, OH, 1992.

General Sources of Physical Data

Daubert, T.E., Danner, R.P., Sibul, H.M., and Stebbins, C.C., *Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation*, extant 1994 (core with 4 supplements), Taylor & Francis, Bristol, PA.

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Physical Constants of Hydrocarbon and Non-Hydrocarbon Compounds, ASTM Data Series DS 4B, ASTM, Philadelphia, 1988.

Riddick, J.A., Bunger, W.B., and Sakano, T.K., *Organic Solvents, Fourth Edition*, John Wiley & Sons, New York, 1986.

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TRC Thermodynamic Tables, Thermodynamic Research Center, Texas A&M University, College Station, TX.

List of Abbreviations

[α], α	specific rotation and column head
∞	soluble in all proportions
ABBIA	*Archives of Biochemistry and Biophysics*
abs	absolute
ac	acid
Ac	acetyl
AC	*Analytical Chemistry*
ace	acetone
$aceD_6$	deuterized acetone
$aceF_6$	hexafluoro acetone
AcOEt	ethyl acetate
Ac_2O	acetic anhydride
ACSAA	*Acta Chemica Scandinavica*
al	alcohol (generally means ethyl alcohol)
ALD	The *Aldrich Handbook of Organic Chemicals and Biochemicals*, Aldrich Chemical Co., Inc., New York; *Aldrich Library of Infrared Spectra*, Aldrich Chemical Co., Milwaukee, WI
ALDN	Aldermaston, *Eight Peak Index of Mass Spectra*, U.K.
alk	alkali
Am	amyl (pentyl)
AmOH	amyl alcohol
amor	amorphous
AMS	*Archives of Mass Spectral Data*, John Wiley & Sons, New York
ANCPA	*Annales de Chimie (Paris)*
anh	anhydrous
API	American Petroleum Institute spectral collection
aq	aqueous
ARKEA	*Arkiv foer Kemi*
b	below
BCSJA	*Bulletin of the Chemical Society of Japan*
Beil Ref	*Beilstein Handbook*
Beil RN	Beilstein Registry Number
BIJOA	*Biochemical Journal*
bipym	bipyramidal
bk	black
bl	blue
BP	boiling point
BPSMA	*Bulletin de l'Academie Polonaise des Sciences*
br	brown
BSCFA	*Bulletin de la Societe Chimique de France*
bt	bright
Bu	butyl
BuOH	butyl alcohol
bz, Bz	benzene
c	percentage concentration
ca	about
CA	*Chemical Abstracts*
CAS	Chemical Abstracts Service
CAS RN	Chemical Abstracts Service Registry Number
CCCCA	*Collection of Czechoslovak Chemical Communications*
cello	cellosolve
CHBEA	*Chemische Berichte*
CHINA	*Chemistry and Industry*
chl, Chl	chloroform
CJCHA	*Canadian Journal of Chemistry*
co	columns
COB	Coblentz Society spectral collection
col	colorless
con, conc	concentrated
COREA	*Comptes Rendus Hebdomaires des Seances de l'Academie des Sciences*
ctc	carbon tetrachloride
cw	continuous wave
cy, cyhex	cyclohexane
cyD_{12}	deuterated cyclohexane
D	589 nm line in the emission spectrum of sodium
DANKA	*Doklady Akademii Nauk S.S.S.R.*
dec	decomposes
DFB	Dollish et al., *Characteristic Raman Frequencies of Organic Compounds*, John Wiley & Sons, New York
dil	dilute
diox	dioxane
dk	dark
dlq	deliquescent
DMF	dimethyl formamide
$DMFD_6$	deuterated dimethyl formamide
efl	efflorescent
Et	ethyl
EtOH	ethyl alcohol
Et_2O	ethyl ether
exp	explodes
fl	flakes
flr	fluorescent
FO	Friedel and Orchin, *Ultraviolet Spectra of Aromatic Compounds*, John Wiley & Sons, New York
FT	Fourier transform
fum	fuming
GCITA	*Gazzetta Chimica Italiana*
gel	gelatinous

gl	glacial
gr	green
gran	granular
gy	gray
HCACA	*Helvetica Chimica Acta*
hex	hexagonal
HOAc	acetic acid
hp	heptane
hx	hexane
hyd	hydrate
hyg	hygroscopic
IJOCA	*Indian Journal of Chemistry*
IR	infrared spectral reference as source of physical constants
irid	iridescent
iso	isooctane
JACSA	*Journal of the American Chemical Society*
JCS,B	*Journal of the Chemical Society, Section B*
JCSOA	*Journal of the Chemical Society (London)*
JJ	Johnson and Jankowski, *Carbon-13 NMR Spectra*, John Wiley & Sons, New York
JMOSA	*Journal of Molecular Spectroscopy*
JOCEA	*Journal of Organic Chemistry*
JPRAA	*Journal de Physique et le Radium*
LA	Levy and Nelson, *Carbon-13 NMR for Organic Chemists*, John Wiley & Sons, New York
LANG	*Absorption Spectra in the UV and Visible Region*, Academic Press, New York
LF	line formula
lf	leaf
lig	ligroin
liq	liquid
lo	long
M	molar concentration
MCA	Manufacturing Chemists Association Research Project, Thermodynamics Research Center, Texas A&M University, College Station, TX
mcl	monoclinic
Me	methyl
MeCN	acetonitrile
MeOH	methyl alcohol
Merck No	Merck Index Monograph number
met	metallic
MF	molecular formula
MOCHA	*Monatshefte für Chemie und Verwandte Teile Anderer Wissenschaften*
mod	modification
MP	melting point
MS	mass spectral reference as source of physical constants
MW	molecular weight
mut	mutarotatory
n	refractive index (n_D), column head
N	normal (concentration of solute in solvent)
nd	needles
NIST	NIST/EPA/MSDC Mass Spectral Database, 1990 Version
NRC	National Research Council spectral collection
oct	octahedral
OES	Phillip et al., *Organic Electronic Spectral Data*, John Wiley & Sons, New York
og	orange
OPSUA	*Optics and Spectroscopy (USSR-English)*
org	organic
orh	orthorhombic
os	organic solvent
pa	pale
par	partial
peth	petroleum ether
Ph	phenyl
PhCl	chlorobenzene
$PhNH_2$	aniline
$PhNO_2$	nitrobenzene
pk	pink
pl	plates
poly D	polysol D
pr	prisms
Pr	propyl
PrOH	propyl alcohol
purp	purple
pwd	powder
py, Py	pyridine
pym	pyramids
pyr, pyrim	pyrimidine
rect	rectangle
res	resinous
rh	rhombic
rhd	rhombohedral
RTCPA	*Recueil des Travaux Chimiques des Pays-Bas*
SAD	Sadtler Research Laboratories spectral collection
SADG	Sadtler Research Laboratories IR grating collection
SADP	Sadtler Research Laboratories IR prism collection
sat	saturated
sl, sli	slight
sol	solid
solu	solution
solv	solvent

SPACA	*Spectrochimica Acta*
st	stable
STOT	Stothers, *Carbon-13 NMR Spectroscopy*, Academic Press, New York
sub	sublimes
sulf	sulfuric acid
syr	syrup
tcl	triclinic
tetr	tetragonal
Tet, TETRA	*Tetrahedron*
tfa	trifluoroacetic acid
thf, THF	tetrahydrofuran
tol	toluene
tr	transparent
trg	trigonal
μ, μm	micron, micrometer; an indicator of an IR spectra converted from micrometers to wavenumbers
undil	undiluted
vac	vacuum
vap	vapor
VAR	Varian Associates NMR spectra collection
vic-	vicinal
visc	viscous
vt	violet
w	water
WILEY	*Atlas of Mass Spectral Data*, John Wiley & Sons, New York
wr	warm
wx	waxy
ye	yellow
xyl	xylene
ZEELA	*Zeitschrift für Elektrochemie*
ZPCBA	*Zeitschrift für Physikalische Chemie, Abteilung B*
ZPCHA	*Zeitschrift für Physiologische Chemie, Hoppe-Seylers*

50-00-0: 5978: Formaldehyde
50-01-1: 6276: Guanidine, monohydrochloride
50-02-2: 9723: Pregna-1,4-diene-3,20-dione, 9-fluoro-11,17,21-trihydroxy-16-methyl-, (11β,16α)-
50-03-3: 9733: Pregn-4-ene-3,20-dione, 21-(acetyloxy)-11,17-dihydroxy-, (11β)-
50-06-6: 11078: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-phenyl-
50-10-2: 5434: Ethanaminium, 2-[(cyclohexylhydroxyphenylacetyl)oxy]-*N*,*N*-diethyl-*N*-methyl-, bromide
50-11-3: 11071: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-diethyl-1-methyl-
50-14-6: 11333: 9,10-Secoergosta-5,7,10(19),22-tetraen-3-ol, (3β,5Z,7E,22E)-
50-22-6: 9734: Pregn-4-ene-3,20-dione, 11,21-dihydroxy-, (11β)-
50-23-7: 9739: Pregn-4-ene-3,20-dione, 11,17,21-trihydroxy-, (11β)-
50-24-8: 9724: Pregna-1,4-diene-3,20-dione, 11,17,21-trihydroxy-, (11β)-
50-27-1: 5395: Estra-1,3,5(10)-triene-3,16,17-triol, (16α,17β)-
50-28-2: 5392: Estra-1,3,5(10)-triene-3,17-diol (17β)-
50-29-3: 2325: Benzene, 1,1'-(2,2,2-trichloroethylidene)bis[4-chloro-
50-30-6: 2561: Benzoic acid, 2,6-dichloro-
50-31-7: 2724: Benzoic acid, 2,3,6-trichloro-
50-32-8: 2392: Benzo[a]pyrene
50-34-0: 9818: 2-Propanaminium, *N*-methyl-*N*-(1-methylethyl)-*N*-[2-[(9H-xanthen-9-ylcarbonyl)oxy]ethyl]-, bromide
50-35-1: 7353: 1H-Isoindole-1,3(2H)-dione, 2-(2,6-dioxo-3-piperidinyl)-
50-36-2: 481: 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, [1*R*-(*exo*,*exo*)]-
50-42-0: 936: Benzeneacetic acid, α-phenyl-, 2-(diethylamino)ethyl ester, hydrochloride
50-44-2: 10746: 6H-Purine-6-thione, 1,7-dihydro-
50-50-0: 5394: Estra-1,3,5(10)-triene-3,17-diol (17β)-, 3-benzoate
50-53-3: 9491: 10H-Phenothiazine-10-propanamine, 2-chloro-*N*,*N*-dimethyl-
50-55-5: 12044: Yohimban-16-carboxylic acid, 11,17-dimethoxy-18-[(3,4,5-trimethoxybenzoyl)oxy]-, methyl ester,
50-69-1: 11328: *D*-Ribose
50-70-4: 6197: *D*-Glucitol
50-71-5: 11056: 2,4,5,6(1H,3H)-Pyrimidinetetrone
50-78-2: 2477: Benzoic acid, 2-(acetyloxy)-
50-79-3: 2559: Benzoic acid, 2,5-dichloro-
50-81-7: 466: *L*-Ascorbic acid
50-82-8: 2725: Benzoic acid, 2,4,5-trichloro-
50-84-0: 2560: Benzoic acid, 2,4-dichloro-
50-85-1: 2628: Benzoic acid, 2-hydroxy-4-methyl-
50-89-5: 11799: Thymidine
50-91-9: 12017: Uridine, 2'-deoxy-5-fluoro-
51-03-6: 9713: Piperonyl butoxide
51-12-7: 10893: 4-Pyridinecarboxylic acid, 2-[3-oxo-3-[(phenylmethyl)amino]propyl]hydrazide
51-17-2: 2373: 1H-Benzimidazole
51-18-3: 11827: 1,3,5-Triazine, 2,4,6-tris(1-aziridinyl)-
51-20-7: 11045: 2,4(1H,3H)-Pyrimidinedione, 5-bromo-
51-21-8: 11050: 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-
51-26-3: 2133: Benzenepropanoic acid, 4-(4-hydroxy-3-iodophenoxy)-3,5-diiodo-
51-28-5: 9327: Phenol, 2,4-dinitro-
51-34-3: 907: Benzeneacetic acid, α-(hydroxymethyl)-, 9-methyl-3-oxa-9-azatricyclo[3.3.1.02,4]non-7-yl ester, [(7S)-(1α,2β,4β,5α,7β)]-
51-35-4: 9753: *L*-Proline, 4-hydroxy-, *trans*-
51-36-5: 2558: Benzoic acid, 3,5-dichloro-
51-41-2: 1498: 1,2-Benzenediol, 4-(2-amino-1-hydroxyethyl)-, (*R*)-
51-43-4: 1519: 1,2-Benzenediol, 4-[1-hydroxy-2-(methylamino)ethyl]-, (*R*)-
51-45-6: 7194: 1H-Imidazole-4-ethanamine
51-48-9: 11913: *L*-Tyrosine, *O*-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-
51-52-5: 11092: 4(1H)-Pyrimidinone, 2,3-dihydro-6-propyl-2-thioxo-
51-55-8: 901: Benzeneacetic acid, α-(hydroxymethyl)- 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester *endo*-(±)-
51-63-8: 1580: Benzeneethanamine, α-methyl-, (*S*)-, sulfate (2:1)
51-66-1: 71: Acetamide, *N*-(4-methoxyphenyl)-
51-67-2: 9194: Phenol, 4-(2-aminoethyl)-
51-75-2: 5404: Ethanamine, 2-chloro-*N*-(2-chloroethyl)-*N*-methyl-
51-79-6: 3941: Carbamic acid, ethyl ester
51-80-9: 7480: Methanediamine, *N*,*N*,*N*',*N*'-tetramethyl-
51-83-2: 5431: Ethanaminium, 2-[(aminocarbonyl)oxy]-*N*,*N*,*N*-trimethyl-, chloride
52-28-8: 7663: Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, (5α,6α)-, phosphate (1:1) (salt)
52-31-3: 11067: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-cyclohexen-1-yl)-5-ethyl-
52-39-1: 9732: Pregn-4-en-18-al, 11,21-dihydroxy-3,20-dioxo-, (11β)-
52-43-7: 11074: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-di-2-propenyl-
52-49-3: 9691: 1-Piperidinepropanol, α-cyclohexyl-α-phenyl-, hydrochloride
52-51-7: 9976: 1,3-Propanediol, 2-bromo-2-nitro-
52-52-8: 4774: Cyclopentanecarboxylic acid, 1-amino-
52-67-5: 12026: *D*-Valine, 3-mercapto-
52-68-6: 11836: Trichlorfon
52-85-7: 5937: Famphur
52-86-8: 3646: 1-Butanone, 4-[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]-1-(4-fluorophenyl)-
52-90-4: 5006: *L*-Cysteine
53-03-2: 9725: Pregna-1,4-diene-3,11,20-trione, 17,21-dihydroxy-
53-05-4: 9730: Pregnane-11,20-dione, 3,17,21-trihydroxy-, (3α,5β)-
53-06-5: 9740: Pregn-4-ene-3,11,20-trione, 17,21-dihydroxy-
53-16-7: 5397: Estra-1,3,5(10)-trien-17-one, 3-hydroxy-
53-41-8: 348: Androstan-17-one, 3-hydroxy-, (3α,5α)-
53-46-3: 5436: Ethanaminium, *N*,*N*-diethyl-*N*-methyl-2-[(9H-xanthen-9-ylcarbonyl)oxy]-, bromide
53-70-3: 5133: Dibenz[a,h]anthracene
53-89-4: 10833: 3H-Pyrazol-3-one, 1,2-dihydro-2-(1-methyl-4-piperidinyl)-5-phenyl-4-(phenylmethyl)-
53-96-3: 64: Acetamide, *N*-9H-fluoren-2-yl-
54-04-6: 1584: Benzeneethanamine, 3,4,5-trimethoxy-
54-06-8: 7291: 1H-Indole-5,6-dione, 2,3-dihydro-3-hydroxy-1-methyl-
54-11-5: 10975: Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (*S*)-
54-25-1: 11815: 1,2,4-Triazine-3,5(2H,4H)-dione, 2-β-*D*-ribofuranosyl-
54-36-4: 10445: 1-Propanone, 2-methyl-1,2-di-3-pyridinyl-
54-85-3: 10888: 4-Pyridinecarboxylic acid, hydrazide
54-95-5: 11637: 5H-Tetrazolo[1,5-a]azepine, 6,7,8,9-tetrahydro-
55-10-7: 895: Benzeneacetic acid, α,4-dihydroxy-3-methoxy-

55-18-5: 5423: Ethanamine, *N*-ethyl-*N*-nitroso-
55-21-0: 599: Benzamide
55-22-1: 10878: 4-Pyridinecarboxylic acid
55-38-9: 5946: Fenthion
55-43-6: 1799: Benzenemethanamine, *N*-(2-chloroethyl)-*N*-(phenylmethyl)-, hydrochloride
55-63-0: 10181: 1,2,3-Propanetriol, trinitrate
55-73-2: 6272: Guanidine, *N,N'*-dimethyl-*N''*-(phenylmethyl)-
55-91-4: 9566: Phosphorofluoridic acid, bis(1-methylethyl) ester
56-03-1: 7224: Imidodicarbonimidic diamide
56-04-2: 11091: 4(1H)-Pyrimidinone, 2,3-dihydro-6-methyl-2-thioxo-
56-12-2: 3460: Butanoic acid, 4-amino-
56-18-8: 9859: 1,3-Propanediamine, *N*-(3-aminopropyl)-
56-23-5: 7530: Methane, tetrachloro-
56-25-7: 5362: 4,7-Epoxyisobenzofuran-1,3-dione, hexahydro-3a,7a-dimethyl-, (3aα,4β,7β,7aα)-
56-29-1: 11066: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-cyclohexen-1-yl)-1,5-dimethyl-
56-33-7: 5229: Disiloxane, 1,1,3,3-tetramethyl-1,3-diphenyl-
56-35-9: 5232: Distannoxane, hexabutyl-
56-36-0: 11521: Stannane, (acetyloxy)tributyl-
56-38-2: 9569: Phosphorothioic acid, *O,O*-diethyl *O*-(4-nitrophenyl) ester
56-40-6: 6241: Glycine
56-41-7: 324: *L*-Alanine
56-45-1: 11339: *L*-Serine
56-49-5: 2388: Benz[j]aceanthrylene, 1,2-dihydro-3-methyl-
56-53-1: 9287: Phenol, 4,4'-(1,2-diethyl-1,2-ethenediyl)bis-, (*E*)-
56-54-2: 4119: Cinchonan-9-ol, 6'-methoxy-, (9*S*)-
56-55-3: 518: Benz[a]anthracene
56-57-5: 11270: Quinoline, 4-nitro-, 1-oxide
56-72-4: 4140: Coumaphos
56-75-7: 52: Acetamide, 2,2-dichloro-*N*-[2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl]-, [*R*-(*R**,*R**)]-
56-81-5: 10170: 1,2,3-Propanetriol
56-82-6: 9768: Propanal, 2,3-dihydroxy-, (±)-
56-84-8: 470: *L*-Aspartic acid
56-85-9: 6240: *L*-Glutamine
56-86-0: 6232: *L*-Glutamic acid
56-87-1: 7409: *L*-Lysine
56-89-3: 5012: *L*-Cystine
57-00-1: 6245: Glycine, *N*-(aminoiminomethyl)-*N*-methyl-
57-06-7: 10558: 1-Propene, 3-isothiocyanato-
57-08-9: 6862: Hexanoic acid, 6-(acetylamino)-
57-10-3: 6635: Hexadecanoic acid
57-11-4: 8237: Octadecanoic acid
57-13-6: 11975: Urea
57-14-7: 7145: Hydrazine, 1,1-dimethyl-
57-15-8: 10390: 2-Propanol, 1,1,1-trichloro-2-methyl-
57-24-9: 11546: Strychnidin-10-one
57-27-2: 7656: Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-methyl- (5α,6α)-
57-41-0: 7210: 2,4-Imidazolidinedione, 5,5-diphenyl-
57-43-2: 11077: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(3-methylbutyl)-
57-44-3: 11070: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-diethyl-
57-47-6: 11174: Pyrrolo[2,3-b]indol-5-ol, 1,2,3,3a,8,8a-hexahydro-1,3a,8-trimethyl-, methylcarbamate (ester), (3a*S-cis*)-
57-50-1: 6209: α-*D*-Glucopyranoside, β-*D*-fructofuranosyl
57-53-4: 10006: 1,3-Propanediol, 2-methyl-2-propyl-, dicarbamate
57-55-6: 9967: 1,2-Propanediol
57-57-8: 8585: 2-Oxetanone
57-62-5: 7694: 2-Naphthacenecarboxamide, 7-chloro-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo, [4S-(4α,4aα,5aα,6β,12aα)]-
57-63-6: 8206: 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17α)-
57-66-9: 2592: Benzoic acid, 4-[(dipropylamino)sulfonyl]-
57-67-0: 2188: Benzenesulfonamide, 4-amino-*N*-(aminoiminomethyl)-
57-68-1: 2193: Benzenesulfonamide, 4-amino-*N*-(4,6-dimethyl-2-pyrimidinyl)-
57-71-6: 3357: 2,3-Butanedione, monooxime
57-74-9: 4070: Chlordane
57-85-2: 359: Androst-4-en-3-one, 17-(1-oxopropoxy)-, (17β)-
57-87-4: 5373: Ergosta-5,7,22-trien-3-ol, (3β,22E)-
57-88-5: 4103: Cholest-5-en-3-ol (3β)-
57-91-0: 5393: Estra-1,3,5(10)-triene-3,17-diol, (17α)-
57-92-1: 11545: Streptomycin
57-97-6: 519: Benz[a]anthracene, 7,12-dimethyl-
58-00-4: 5146: 4H-Dibenzo[de,g]quinoline-10,11-diol, 5,6,6a,7-tetrahydro-6-methyl-, (*R*)-
58-05-9: 6235: *L*-Glutamic acid, *N*-[4-[[(2-amino-5-formyl-1,4,5,6,7,8-hexahydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]-
58-08-2: 10743: 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-
58-14-0: 11034: 2,4-Pyrimidinediamine, 5-(4-chlorophenyl)-6-ethyl-
58-15-1: 10834: 3H-Pyrazol-3-one, 4-(dimethylamino)-1,2-dihydro-1,5-dimethyl-2-phenyl-
58-18-4: 358: Androst-4-en-3-one, 17-hydroxy-17-methyl-, (17β)-
58-22-0: 356: Androst-4-en-3-one, 17-hydroxy-, (17β)-
58-25-3: 2406: 3H-1,4-Benzodiazepin-2-amine, 7-chloro-*N*-methyl-5-phenyl-, 4-oxide
58-27-5: 7854: 1,4-Naphthalenedione, 2-methyl-
58-32-2: 5702: Ethanol, 2,2',2'',2'''-[(4,8-di-1-piperidinylpyrimido[5,4-d]pyrimidine-
58-38-8: 9487: 10H-Phenothiazine, 2-chloro-10-[3-(4-methyl-1-piperazinyl)propyl]-
58-39-9: 9603: 1-Piperazineethanol, 4-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-
58-46-8: 2393: 2H-Benzo[a]quinolizin-2-one, 1,3,4,6,7,11b-hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-
58-54-8: 168: Acetic acid, [2,3-dichloro-4-(2-methylene-1-oxobutyl)phenoxy]-
58-55-9: 10739: 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-
58-56-0: 10917: 3,4-Pyridinedimethanol, 5-hydroxy-6-methyl-, hydrochloride
58-61-7: 319: Adenosine
58-63-9: 7325: Inosine
58-72-0: 1646: Benzene, 1,1',1''-(1-ethenyl-2-ylidene)tris-
58-73-1: 5413: Ethanamine, 2-(diphenylmethoxy)-*N,N*-dimethyl-
58-74-2: 7368: Isoquinoline, 1-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxy-
58-85-5: 11672: 1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, [3a*S*-(3aα,4β,6aα)]-
58-86-6: 12042: *D*-Xylose
58-89-9: 4401: Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1α,2α,3β,4α,5α,6β)-
58-90-2: 9456: Phenol, 2,3,4,6-tetrachloro-
58-93-5: 2855: 2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3,4-dihydro-, 1,1-dioxide
58-94-6: 2853: 2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-, 1,1-dioxide
58-95-7: 2784: 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, acetate, [2*R*-[2*R**(4*R**,8*R**
58-96-8: 12016: Uridine

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58-97-9: 12018: 5'-Uridylic acid
59-00-7: 11213: 2-Quinolinecarboxylic acid, 4,8-dihydroxy-
59-02-9: 2785: 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2*R*-[2*R**(4*R**,8*R**)]]-
59-23-4: 6188: *D*-Galactose
59-26-7: 10875: 3-Pyridinecarboxamide, *N,N*-diethyl-
59-30-3: 6234: *L*-Glutamic acid, *N*-[4-[[(2-amino-1,4-dihydro-4-oxo-6-pteridinyl)methyl]amino] benzoyl]-
59-31-4: 11308: 2(1H)-Quinolinone
59-40-5: 2202: Benzenesulfonamide, 4-amino-*N*-2-quinoxalinyl-
59-46-1: 2490: Benzoic acid, 4-amino-, 2-(diethylamino)ethyl ester
59-47-2: 10004: 1,2-Propanediol, 3-(2-methylphenoxy)-
59-48-3: 7317: 2H-Indol-2-one, 1,3-dihydro-
59-49-4: 2879: 2(3H)-Benzoxazolone
59-50-7: 9247: Phenol, 4-chloro-3-methyl-
59-51-8: 7638: *DL*-Methionine
59-52-9: 10353: 1-Propanol, 2,3-dimercapto-
59-66-5: 32: Acetamide, *N*-[5-(aminosulfonyl)-1,3,4-thiadiazol-2-yl]-
59-67-6: 10877: 3-Pyridinecarboxylic acid
59-87-0: 7135: Hydrazinecarboxamide, 2-[(5-nitro-2-furanyl)methylene]-
59-88-1: 7163: Hydrazine, phenyl-, monohydrochloride
59-89-2: 7689: Morpholine, 4-nitroso-
59-92-7: 11912: *L*-Tyrosine, 3-hydroxy-
59-98-3: 7189: 1H-Imidazole, 4,5-dihydro-2-(phenylmethyl)-
60-00-4: 6253: Glycine, *N,N'*-1,2-ethanediylbis[*N*-(carboxymethyl)-
60-01-5: 3581: Butanoic acid, 1,2,3-propanetriyl ester
60-09-3: 836: Benzenamine, 4-(phenylazo)-
60-10-6: 5113: Diazenecarbothioic acid, phenyl-, 2-phenylhydrazide
60-11-7: 721: Benzenamine, *N,N*-dimethyl-4-(phenylazo)-
60-12-8: 1590: Benzeneethanol
60-18-4: 11909: *L*-Tyrosine
60-23-1: 5640: Ethanethiol, 2-amino-
60-24-2: 5723: Ethanol, 2-mercapto-
60-27-5: 7221: 4H-Imidazol-4-one, 2-amino-1,5-dihydro-1-methyl-
60-29-7: 5599: Ethane, 1,1'-oxybis-
60-31-1: 5430: Ethanaminium, 2-(acetyloxy)-*N,N,N*-trimethyl-, chloride
60-32-2: 6864: Hexanoic acid, 6-amino-
60-33-3: 8214: 9,12-Octadecadienoic acid (*Z,Z*)-
60-34-4: 7152: Hydrazine, methyl-
60-35-5: 22: Acetamide
60-41-3: 11549: Strychnidin-10-one, sulfate (2:1)
60-51-5: 5001: Cygon
60-54-8: 7696: 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-,[4S-(4α,4aα,5aα,6β,12aα)]-
60-56-0: 7205: 2*H*-Imidazole-2-thione, 1,3-dihydro-1-methyl-
60-57-1: 5169: 2,7:3,6-Dimethanonaphth[2,3-b]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aα,2β,2aα,3β,6β,6aα,7β,7aα)-
60-70-8: 12027: Veratraman-3,23-diol, 14,15,16,17-tetradehydro-, (3β,23β)-
60-80-0: 10830: 3H-Pyrazol-3-one, 1,2-dihydro-1,5-dimethyl-2-phenyl-
60-82-2: 10436: 1-Propanone, 3-(4-hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-
60-87-7: 9490: 10H-Phenothiazine-10-ethanamine, *N,N*,α-trimethyl-
60-91-3: 9489: 10H-Phenothiazine-10-ethanamine, *N,N*-diethyl-
61-00-7: 5798: Ethanone, 1-[10-[3-(dimethylamino)propyl]-10*H*-phenothiazin-2-yl]-
61-12-1: 11209: 4-Quinolinecarboxamide, 2-butoxy-*N*-[2-(diethylamino)ethyl]-, monohydrochloride
61-19-8: 320: 5'-Adenylic acid
61-50-7: 7293: 1H-Indole-3-ethanamine, *N,N*-dimethyl-
61-54-1: 7292: 1H-Indole-3-ethanamine
61-73-4: 9492: Phenothiazin-5-ium, 3,7-bis(dimethylamino)-, chloride
61-78-9: 6243: Glycine, *N*-(4-aminobenzoyl)-
61-80-3: 2873: 2-Benzoxazolamine, 5-chloro-
61-82-5: 11828: 1H-1,2,4-Triazol-3-amine
61-90-5: 7403: *L*-Leucine
62-23-7: 2701: Benzoic acid, 4-nitro-
62-38-4: 7421: Mercury, (acetato-*O*)phenyl-
62-44-2: 60: Acetamide, *N*-(4-ethoxyphenyl)-
62-50-0: 7521: Methanesulfonic acid, ethyl ester
62-51-1: 9816: 1-Propanaminium, 2-(acetyloxy)-*N,N,N*-trimethyl-, chloride
62-53-3: 632: Benzenamine
62-54-4: 122: Acetic acid, calcium salt
62-55-5: 5634: Ethanethioamide
62-56-6: 11782: Thiourea
62-57-7: 331: Alanine, 2-methyl-
62-59-9: 4062: Cevane-3,4,12,14,16,17,20-heptol, 4,9-epoxy-, 3-(2-methyl-2-butenoate), [3β(*Z*),4α,16β]-
62-73-7: 5161: Dichlorvos
62-75-9: 7440: Methanamine, *N*-methyl-*N*-nitroso-
62-76-0: 5557: Ethanedioic acid, disodium salt
62-90-8: 5399: Estr-4-en-3-one, 17-(1-oxo-3-phenylpropoxy)-, (17β)-
63-05-8: 352: Androst-4-ene-3,17-dione
63-25-2: 8022: 1-Naphthalenol, methylcarbamate
63-68-3: 7637: *L*-Methionine
63-74-1: 2184: Benzenesulfonamide, 4-amino-
63-75-2: 10896: 3-Pyridinecarboxylic acid, 1,2,5,6-tetrahydro-1-methyl-, methyl ester
63-91-2: 9495: *L*-Phenylalanine
63-98-9: 878: Benzeneacetamide, *N*-(aminocarbonyl)-
64-04-0: 1567: Benzeneethanamine
64-10-8: 12009: Urea, phenyl-
64-17-5: 5663: Ethanol
64-18-6: 5993: Formic acid
64-19-7: 100: Acetic acid
64-20-0: 7446: Methanaminium, *N,N,N*-trimethyl-, bromide
64-65-3: 9642: 2,6-Piperidinedione, 4-ethyl-4-methyl-
64-67-5: 11556: Sulfuric acid, diethyl ester
64-69-7: 200: Acetic acid, iodo-
64-77-7: 2204: Benzenesulfonamide, *N*-[(butylamino)carbonyl]-4-methyl-
64-85-7: 9736: Pregn-4-ene-3,20-dione, 21-hydroxy-
64-86-8: 93: Acetamide, *N*-(5,6,7,9-tetrahydro-1,2,3,10-tetramethoxy-9-oxobenzo[a]heptalen-7-yl)-, (*S*)-
65-29-2: 5432: Ethanaminium, 2,2',2"-[1,2,3-benzenetriyltris(oxy)]tris[*N,N,N*-triethyl-, tr
65-45-2: 615: Benzamide, 2-hydroxy-
65-46-3: 5013: Cytidine
65-49-6: 2496: Benzoic acid, 4-amino-2-hydroxy-
65-64-5: 7161: Hydrazine, (1-phenylethyl)-
65-71-4: 11052: 2,4(1H,3H)-Pyrimidinedione, 5-methyl-
65-82-7: 7639: *L*-Methionine, *N*-acetyl-
65-85-0: 2472: Benzoic acid
65-86-1: 11033: 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-
66-02-4: 11911: Tyrosine, 3,5-diiodo-
66-22-8: 11042: 2,4(1H,3H)-Pyrimidinedione
66-23-9: 5429: Ethanaminium, 2-(acetyloxy)-*N,N,N*-trimethyl-, bromide
66-25-1: 6709: Hexanal

75-25-2: 7538: Methane, tribromo-
75-26-3: 9822: Propane, 2-bromo-
75-27-4: 7457: Methane, bromodichloro-
75-28-5: 10057: Propane, 2-methyl-
75-29-6: 9834: Propane, 2-chloro-
75-30-9: 10039: Propane, 2-iodo-
75-31-0: 9790: 2-Propanamine
75-33-2: 10140: 2-Propanethiol
75-34-3: 5519: Ethane, 1,1-dichloro-
75-35-4: 5885: Ethene, 1,1-dichloro-
75-36-5: 294: Acetyl chloride
75-37-6: 5536: Ethane, 1,1-difluoro-
75-38-7: 5893: Ethene, 1,1-difluoro-
75-39-8: 5665: Ethanol, 1-amino-
75-43-4: 7492: Methane, dichlorofluoro-
75-44-5: 4000: Carbonic dichloride
75-45-6: 7468: Methane, chlorodifluoro-
75-46-7: 7548: Methane, trifluoro-
75-47-8: 7550: Methane, triiodo-
75-50-3: 7434: Methanamine, *N,N*-dimethyl-
75-52-5: 7512: Methane, nitro-
75-54-7: 11381: Silane, dichloromethyl-
75-55-8: 499: Aziridine, 2-methyl-
75-57-0: 7447: Methanaminium, *N,N,N*-trimethyl-, chloride
75-58-1: 7448: Methanaminium, *N,N,N*-trimethyl-, iodide
75-60-5: 451: Arsinic acid, dimethyl-
75-61-6: 7486: Methane, dibromodifluoro-
75-62-7: 7464: Methane, bromotrichloro-
75-63-8: 7465: Methane, bromotrifluoro-
75-64-9: 9804: 2-Propanamine, 2-methyl-
75-65-0: 10371: 2-Propanol, 2-methyl-
75-66-1: 10142: 2-Propanethiol, 2-methyl-
75-68-3: 5462: Ethane, 1-chloro-1,1-difluoro
75-69-4: 7545: Methane, trichlorofluoro-
75-71-8: 7490: Methane, dichlorodifluoro-
75-72-9: 7476: Methane, chlorotrifluoro-
75-73-0: 7531: Methane, tetrafluoro-
75-74-1: 9718: Plumbane, tetramethyl
75-75-2: 7520: Methanesulfonic acid
75-76-3: 11434: Silane, tetramethyl-
75-77-4: 11372: Silane, chlorotrimethyl-
75-78-5: 11377: Silane, dichlorodimethyl-
75-79-6: 11448: Silane, trichloromethyl-
75-80-9: 5758: Ethanol, 2,2,2-tribromo-
75-81-0: 5511: Ethane, 1,2-dibromo-1,1-dichloro-
75-82-1: 5513: Ethane, 1,2-dibromo-1,1-difluoro-
75-83-2: 3287: Butane, 2,2-dimethyl-
75-84-3: 10356: 1-Propanol, 2,2-dimethyl-
75-85-4: 3621: 2-Butanol, 2-methyl-
75-86-5: 10092: Propanenitrile, 2-hydroxy-2-methyl-
75-87-6: 21: Acetaldehyde, trichloro-
75-88-7: 5478: Ethane, 2-chloro-1,1,1-trifluoro-
75-89-8: 5761: Ethanol, 2,2,2-trifluoro-
75-91-2: 7169: Hydroperoxide, 1,1-dimethylethyl
75-93-4: 11560: Sulfuric acid, monomethyl ester
75-94-5: 11444: Silane, trichloroethenyl-
75-95-6: 5607: Ethane, pentabromo-
75-96-7: 241: Acetic acid, tribromo-
75-97-8: 3652: 2-Butanone, 3,3-dimethyl-
75-98-9: 10242: Propanoic acid, 2,2-dimethyl-
75-99-0: 10228: Propanoic acid, 2,2-dichloro-
76-00-6: 10389: 2-Propanol, 1,1,1-trichloro-
76-01-7: 5608: Ethane, pentachloro-
76-02-8: 300: Acetyl chloride, trichloro-
76-03-9: 243: Acetic acid, trichloro-
76-04-0: 127: Acetic acid, chlorodifluoro-
76-05-1: 263: Acetic acid, trifluoro-
76-06-2: 7547: Methane, trichloronitro-
76-08-4: 10388: 2-Propanol, 1,1,1-tribromo-2-methyl-
76-09-5: 3345: 2,3-Butanediol, 2,3-dimethyl-
76-11-9: 5628: Ethane, 1,1,1,2-tetrachloro-2,2-difluoro-
76-12-0: 5627: Ethane, 1,1,2,2-tetrachloro-1,2-difluoro-
76-13-1: 5654: Ethane, 1,1,2-trichloro-1,2,2-trifluoro-
76-14-2: 5529: Ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-
76-15-3: 5475: Ethane, chloropentafluoro-
76-16-4: 5587: Ethane, hexafluoro-
76-17-5: 10165: Propane, 1,2,3-trichloro-1,1,2,3,3-pentafluoro-
76-19-7: 10102: Propane, octafluoro-
76-20-0: 3227: Butane, 2,2-bis(ethylsulfonyl)-
76-24-4: 3103: [5,5'-Bipyrimidine]-2,2',4,4',6,6'(1H,1'H,3H,3'H,5H,5'H)-hexone-5,5'-dihydroxy
76-28-8: 4040: Card-20(22)-enolide, 3,11,14-trihydroxy-, (3β,5β,11α)-
76-30-2: 3338: Butanedioic acid, tetrahydroxy-
76-36-8: 3188: Butanal, 2,2,3-trichloro-
76-37-9: 10387: 1-Propanol, 2,2,3,3-tetrafluoro-
76-39-1: 10374: 1-Propanol, 2-methyl-2-nitro-
76-43-7: 355: Androst-4-en-3-one, 9-fluoro-11,17-dihydroxy-17-methyl-, (11β,17β)-
76-44-8: 7566: 4,7-Methano-1H-indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-
76-45-9: 4063: Cevane-3,4,6,7,14,15,16,20-octol, 4,9-epoxy-, (3β,4α,6α,7α,15α,16β
76-49-3: 2941: Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate, *endo*-
76-57-3: 7662: Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, (5α,6α)-
76-59-5: 9353: Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-3-methyl-6-(1-methylethyl)-, *S,S*-dioxide
76-60-8: 9350: Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-3-methyl-, *S,S*-dioxide
76-61-9: 9355: Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[5-methyl-2-(1-methylethyl)-, *S,S*-dioxide
76-62-0: 7340: 1(3H)-Isobenzofuranone, 3,3-bis(3,5-dibromo-4-hydroxyphenyl)-
76-65-3: 2460: 2(3H)-Benzofuranone, 3-[2-(diethylamino)ethyl]-3-phenyl-
76-67-5: 9937: Propanedioic acid, ethylphenyl-, diethyl ester
76-68-6: 11068: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2-cyclopenten-1-yl)-5-(2-propenyl)-
76-76-6: 11075: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(1-methylethyl)-
76-80-2: 3107: 3H-Bis[1]benzopyrano[3,4-b:6',5'-e]pyran-7(7aH)-one, 13,13a-dihydro-7a-hydroxy-9,10-dimethoxy-3,3-dimethyl
76-83-5: 1194: Benzene, 1,1',1"-(chloromethylidyne)tris-
76-84-6: 1864: Benzenemethanol, α,α-diphenyl-
76-87-9: 11894: Triphenyltin hydroxide
76-89-1: 918: Benzeneacetic acid, α-hydroxy-α-phenyl-, methyl ester
76-93-7: 916: Benzeneacetic acid, α-hydroxy-α-phenyl-
76-94-8: 11083: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-methyl-5-phenyl-
77-02-1: 11081: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylethyl)-5-(2-propenyl)-
77-03-2: 9640: 2,4-Piperidinedione, 3,3-diethyl-
77-04-3: 10929: 2,4(1H,3H)-Pyridinedione, 3,3-diethyl-
77-06-5: 6195: Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone,
77-09-8: 7342: 1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxyphenyl)-
77-10-1: 9682: Piperidine, 1-(1-phenylcyclohexyl)-

77-16-7: 11887: 2H,4aH-1,4,5-Trioxadicyclopent[a,hi]indene-7-carboxylic acid, 3-ethylidene-3,3a,7a,9b-tetrahydro-2-oxo-, methyl ester, [3aS-(3E,3aα,4aβ,7aβ,9aR*,9bβ)]-
77-25-8: 9925: Propanedioic acid, diethyl-, diethyl ester
77-26-9: 11084: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2-methylpropyl)-5-(2-propenyl)-
77-28-1: 11065: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-butyl-5-ethyl-
77-40-7: 9419: Phenol, 4,4'-(1-methylpropylidene)bis-
77-41-8: 11139: 2,5-Pyrrolidinedione, 1,3-dimethyl-3-phenyl-
77-42-9: 9090: 2-Penten-1-ol, 2-methyl-5-(2-methyl-3-methylenebicyclo[2.2.1]hept-2-yl)-, [1*S*-[1α,2α(*Z*),4α]
77-46-3: 91: Acetamide, *N,N'*-(sulfonyldi-4,1-phenylene)bis-
77-47-4: 4758: 1,3-Cyclopentadiene, 1,2,3,4,5,5-hexachloro-
77-48-5: 7208: 2,4-Imidazolidinedione, 1,3-dibromo-5,5-dimethyl-
77-49-6: 10003: 1,3-Propanediol, 2-methyl-2-nitro-
77-52-1: 12020: Urs-12-en-28-oic acid, 3-hydroxy-, (3β)-
77-53-2: 7560: 1H-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-,
77-59-8: 11511: Spirosolan-3-ol, (3β,5α,22β,25*S*)-
77-60-1: 11515: Spirostan-3-ol, (3β,5α,25*R*)-
77-63-4: 4991: Cyclotetrasiloxane, 2,4,6,8-tetramethyl-2,4,6,8-tetraphenyl-
77-65-6: 3192: Butanamide, *N*-(aminocarbonyl)-2-bromo-2-ethyl-
77-67-8: 11141: 2,5-Pyrrolidinedione, 3-ethyl-3-methyl-
77-71-4: 7209: 2,4-Imidazolidinedione, 5,5-dimethyl-
77-74-7: 8926: 3-Pentanol, 3-methyl-
77-75-8: 9133: 1-Pentyn-3-ol, 3-methyl-
77-76-9: 9894: Propane, 2,2-dimethoxy-
77-77-0: 5904: Ethene, 1,1'-sulfonylbis-
77-78-1: 11557: Sulfuric acid, dimethyl ester
77-79-2: 11735: Thiophene, 2,5-dihydro-, 1,1-dioxide
77-83-8: 8594: Oxiranecarboxylic acid, 3-methyl-3-phenyl-, ethyl ester
77-84-9: 9992: 1,3-Propanediol, 2-ethyl-2-methyl-
77-85-0: 9996: 1,3-Propanediol, 2-(hydroxymethyl)-2-methyl-
77-86-1: 9971: 1,3-Propanediol, 2-amino-2-(hydroxymethyl)-
77-89-4: 10150: 1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, triethyl ester
77-92-9: 10152: 1,2,3-Propanetricarboxylic acid, 2-hydroxy-
77-93-0: 10154: 1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester
77-94-1: 10153: 1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tributyl ester
77-95-2: 4330: Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1*R*-(1α,3α,4α,5β)]-
77-99-6: 9991: 1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-
78-00-2: 9717: Plumbane, tetraethyl
78-07-9: 11461: Silane, triethoxyethyl-
78-08-0: 11407: Silane, ethenyltriethoxy-
78-09-1: 5592: Ethane, 1,1',1",1'"-[methanetetrayltetrakis(oxy)] tetrakis-
78-10-4: 11489: Silicic acid (H4SiO4), tetraethyl ester
78-11-5: 9975: 1,3-Propanediol, 2,2-bis[(nitrooxy)methyl]-, dinitrate (ester)
78-13-7: 11490: Silicic acid (H4SiO4), tetrakis(2-ethylbutyl) ester
78-26-2: 10005: 1,3-Propanediol, 2-methyl-2-propyl-
78-27-3: 4521: Cyclohexanol, 1-ethynyl-
78-30-8: 9555: Phosphoric acid, tris(2-methylphenyl) ester
78-32-0: 9557: Phosphoric acid, tris(4-methylphenyl) ester
78-34-2: 5192: Dioxathion
78-38-6: 9522: Phosphonic acid, ethyl-, diethyl ester
78-39-7: 5655: Ethane, 1,1,1-triethoxy-
78-40-0: 9549: Phosphoric acid, triethyl ester
78-48-8: 11835: *S,S,S*-Tributyl phosphorotrothioate
78-54-6: 4520: Cyclohexanol, 1,1'-(1,2-ethynediyl)bis-
78-59-1: 4714: 2-Cyclohexen-1-one, 3,5,5-trimethyl-
78-62-6: 11388: Silane, diethoxydimethyl-
78-67-1: 10077: Propanenitrile, 2,2'-azobis[2-methyl-
78-74-0: 5644: Ethane, 1,1,2-tribromo-
78-75-1: 9865: Propane, 1,2-dibromo-
78-77-3: 9831: Propane, 1-bromo-2-methyl-
78-78-4: 3393: Butane, 2-methyl-
78-79-5: 3168: 1,3-Butadiene, 2-methyl-
78-80-8: 3885: 1-Buten-3-yne, 2-methyl-
78-81-9: 9803: 1-Propanamine, 2-methyl-
78-82-0: 10095: Propanenitrile, 2-methyl-
78-83-1: 10372: 1-Propanol, 2-methyl-
78-84-2: 9771: Propanal, 2-methyl-
78-85-3: 10498: 2-Propenal, 2-methyl-
78-88-6: 10535: 1-Propene, 2,3-dichloro-
78-89-7: 10330: 1-Propanol, 2-chloro-
78-92-2: 3589: 2-Butanol
78-93-3: 3640: 2-Butanone
78-94-4: 3869: 3-Buten-2-one
78-95-5: 10403: 2-Propanone, 1-chloro-
78-97-7: 10089: Propanenitrile, 2-hydroxy-
78-98-8: 9774: Propanal, 2-oxo-
78-99-9: 9879: Propane, 1,1-dichloro-
79-00-5: 5647: Ethane, 1,1,2-trichloro-
79-01-6: 5913: Ethene, trichloro-
79-03-8: 10476: Propanoyl chloride
79-04-9: 295: Acetyl chloride, chloro-
79-05-0: 9777: Propanamide
79-06-1: 10502: 2-Propenamide
79-07-2: 41: Acetamide, 2-chloro-
79-08-3: 111: Acetic acid, bromo-
79-09-4: 10185: Propanoic acid
79-10-7: 10592: 2-Propenoic acid
79-11-8: 123: Acetic acid, chloro-
79-14-1: 196: Acetic acid, hydroxy-
79-15-2: 36: Acetamide, *N*-bromo-
79-16-3: 72: Acetamide, *N*-methyl-
79-17-4: 7138: Hydrazinecarboximidamide
79-19-6: 7133: Hydrazinecarbothioamide
79-20-9: 208: Acetic acid, methyl ester
79-21-0: 5610: Ethaneperoxoic acid
79-22-1: 4016: Carbonochloridic acid, methyl ester
79-24-3: 5598: Ethane, nitro-
79-27-6: 5622: Ethane, 1,1,2,2-tetrabromo-
79-28-7: 5905: Ethene, tetrabromo-
79-29-8: 3286: Butane, 2,3-dimethyl-
79-30-1: 10487: Propanoyl chloride, 2-methyl-
79-31-2: 10273: Propanoic acid, 2-methyl-
79-34-5: 5625: Ethane, 1,1,2,2-tetrachloro-
79-35-6: 5888: Ethene, 1,1-dichloro-2,2-difluoro-
79-36-7: 297: Acetyl chloride, dichloro-
79-37-8: 5576: Ethanedioyl dichloride
79-38-9: 5880: Ethene, chlorotrifluoro-
79-40-3: 5579: Ethanedithioamide
79-41-4: 10631: 2-Propenoic acid, 2-methyl-
79-43-6: 162: Acetic acid, dichloro-

79-44-7: 3966: Carbamic chloride, dimethyl-
79-46-9: 10101: Propane, 2-nitro-
79-49-2: 10460: 2-Propanone, 1,1,1,3,3-pentabromo-
79-53-8: 10404: 2-Propanone, 1-chloro-1,1,3,3,3-pentafluoro-
79-54-9: 9153: 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1α,4aβ,4bα,10aα)]-
79-55-0: 9677: Piperidine, 1,2,2,6,6-pentamethyl-
79-57-2: 7695: 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,5,6,10,12,12a-hexahydroxy-6-methyl-1,11-dioxo-,[4S-(4α,4aα,5aα,6β,12aα)]-
79-58-3: 11498: Solanid-5-ene-3,12-diol, (3β,12α)-
79-63-0: 7401: Lanosta-8,24-dien-3-ol, (3β)-
79-69-6: 3877: 3-Buten-2-one, 4-(2,5,6,6-tetramethyl-2-cyclohexen-1-yl)-
79-70-9: 3876: 3-Buten-2-one, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-
79-74-3: 1499: 1,4-Benzenediol, 2,5-bis(1,1-dimethylpropyl)-
79-77-6: 3878: 3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (*E*)-
79-83-4: 329: β-Alanine, *N*-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-, (*R*)-
80-00-2: 1223: Benzene, 1-chloro-4-(phenylsulfonyl)-
80-05-7: 9399: Phenol, 4,4'-(1-methylethylidene)bis-
80-06-8: 1848: Benzenemethanol, 4-chloro-α-(4-chlorophenyl)-α-methyl-
80-07-9: 2236: Benzene, 1,1'-sulfonylbis[4-chloro-
80-08-0: 845: Benzenamine, 4,4'-sulfonylbis-
80-09-1: 9452: Phenol, 4,4'-sulfonylbis-
80-10-4: 11378: Silane, dichlorodiphenyl-
80-11-5: 2209: Benzenesulfonamide, *N*,4-dimethyl-*N*-nitroso-
80-13-7: 2562: Benzoic acid, 4-[(dichloroamino)sulfonyl]-
80-14-8: 11898: Trisiloxane, 1,1,3,5,5-pentamethyl-1,3,5-triphenyl-
80-15-9: 7172: Hydroperoxide, 1-methyl-1-phenylethyl
80-18-2: 2225: Benzenesulfonic acid, methyl ester
80-26-2: 4661: 3-Cyclohexene-1-methanol, α,α,4-trimethyl-, acetate
80-32-0: 2190: Benzenesulfonamide, 4-amino-*N*-(6-chloro-3-pyridazinyl)-
80-33-1: 2218: Benzenesulfonic acid, 4-chloro-, 4-chlorophenyl ester
80-35-3: 2196: Benzenesulfonamide, 4-amino-*N*-(6-methoxy-3-pyridazinyl)-
80-40-0: 2224: Benzenesulfonic acid, 4-methyl-, ethyl ester
80-42-2: 2232: Benzenesulfonic acid, propyl ester
80-46-6: 9325: Phenol, 4-(1,1-dimethylpropyl)-
80-48-8: 2227: Benzenesulfonic acid, 4-methyl-, methyl ester
80-55-7: 10257: Propanoic acid, 2-hydroxy-2-methyl-, ethyl ester
80-56-8: 2971: Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl
80-59-1: 3838: 2-Butenoic acid, 2-methyl-, (*E*)-
80-62-6: 10646: 2-Propenoic acid, 2-methyl-, methyl ester
80-63-7: 10604: 2-Propenoic acid, 2-chloro-, methyl ester
80-69-3: 9941: Propanedioic acid, hydroxy-
80-72-8: 4934: 2-Cyclopenten-1-one, 2,3-dihydroxy-
80-92-2: 9728: Pregnane-3,20-diol, (3α,5β,20*S*)-
80-97-7: 4100: Cholestanol
81-04-9: 7866: 1,5-Naphthalenedisulfonic acid
81-07-2: 2385: 1,2-Benzisothiazol-3(2H)-one, 1,1-dioxide
81-08-3: 2872: 3H-2,1-Benzoxathiol-3-one, 1,1-dioxide
81-13-0: 3199: Butanamide, 2,4-dihydroxy-*N*-(3-hydroxypropyl)-3,3-dimethyl-, (*R*)-
81-15-2: 1459: Benzene, 1-(1,1-dimethylethyl)-3,5-dimethyl-2,4,6-trinitro-
81-16-3: 7953: 1-Naphthalenesulfonic acid, 2-amino-
81-20-9: 1475: Benzene, 1,3-dimethyl-2-nitro-
81-23-2: 4094: Cholan-24-oic acid, 3,7,12-trioxo-, (5β)-
81-24-3: 5616: Ethanesulfonic acid, 2-[[(3α,5β,7α,12α)-3,7,12-trihydroxy-24-oxocholan-24-yl]amino]-
81-25-4: 4093: Cholan-24-oic acid, 3,7,12-trihydroxy-, (3α,5β,7α,12α)-
81-30-1: 2781: [2]Benzopyrano[6,5,4-def][2]benzopyran-1,3,6,8-tetrone
81-38-9: 2467: 5H-Benzo[g]-1,3-benzodioxolo[6,5,4-de]quinoline, 6,7,7a,8-tetrahydro-11-methoxy-7-methyl-, (*R*)-
81-54-9: 419: 9,10-Anthracenedione, 1,2,4-trihydroxy-
81-61-8: 414: 9,10-Anthracenedione, 1,2,5,8-tetrahydroxy-
81-64-1: 396: 9,10-Anthracenedione, 1,4-dihydroxy-
81-77-6: 434: 5,9,14,18-Anthrazinetetrone, 6,15-dihydro-
81-81-2: 2829: 2H-1-Benzopyran-2-one, 4-hydroxy-3-(3-oxo-1-phenylbutyl)-
81-88-9: 12039: Xanthylium, 9-(2-carboxyphenyl)-3,6-bis(diethylamino)-, chloride
81-90-3: 2514: Benzoic acid, 2-[bis(4-hydroxyphenyl)methyl]-
81-92-5: 1839: Benzenemethanol, 2-[bis(4-hydroxyphenyl)methyl]-
82-02-0: 6176: 5H-Furo[3,2-g][1]benzopyran-5-one, 4,9-dimethoxy-7-methyl-
82-05-3: 6283: 7H-Benz[de]anthracen-7-one
82-12-2: 406: 9,10-Anthracenedione, 1,2,3,5,6,7-hexahydroxy-
82-28-0: 384: 9,10-Anthracenedione, 1-amino-2-methyl-
82-29-1: 417: 9,10-Anthracenedione, 1,2,6-trihydroxy-
82-34-8: 410: 9,10-Anthracenedione, 1-nitro-
82-35-9: 405: 9,10-Anthracenedione, 1,5-dinitro-
82-40-6: 6173: Furo[2,3-b]quinolin-4(2H)-one, 3,9-dihydro-8-methoxy-9-methyl-2-(1-methylethyl)-, (*R*)-
82-44-0: 388: 9,10-Anthracenedione, 1-chloro-
82-45-1: 381: 9,10-Anthracenedione, 1-amino-
82-54-2: 5207: 1,3-Dioxolo[4,5-g]isoquinolin-5-ol, 5,6,7,8-tetrahydro-4-methoxy-6-methyl-
82-57-5: 6179: 5H-Furo[3,2-g][1]benzopyran-5-one, 4-methoxy-7-methyl-
82-58-6: 5367: Ergoline-8-carboxylic acid, 9,10-didehydro-6-methyl-, (8β)-
82-62-2: 9476: Phenol, 3,4,6-trichloro-2-nitro-
82-66-6: 7258: 1H-Indene-1,3(2H)-dione, 2-(diphenylacetyl)-
82-68-8: 2084: Benzene, pentachloronitro-
82-71-3: 1552: 1,3-Benzenediol, 2,4,6-trinitro-
82-75-7: 7957: 1-Naphthalenesulfonic acid, 8-amino-
82-86-0: 8: 1,2-Acenaphthylenedione
83-07-8: 10828: 3H-Pyrazol-3-one, 4-amino-1,2-dihydro-1,5-dimethyl-2-phenyl-
83-12-5: 7260: 1H-Indene-1,3(2H)-dione, 2-phenyl-
83-13-6: 9960: Propanedioic acid, phenyl-, diethyl ester
83-14-7: 7384: 8-Isoquinolinol, 1,2,3,4-tetrahydro-6,7-dimethoxy-1,2-dimethyl-, (*S*)-
83-25-0: 11145: 2,5-Pyrrolidinedione, 1-phenyl-

83-27-2: 9953: Propanedioic acid, (1-methylpropyl)-, diethyl ester
83-32-9: 6: Acenaphthylene, 1,2-dihydro-
83-33-0: 7276: 1H-Inden-1-one, 2,3-dihydro-
83-34-1: 7305: 1H-Indole, 3-methyl-
83-40-9: 2626: Benzoic acid, 2-hydroxy-3-methyl-
83-41-0: 1477: Benzene, 1,2-dimethyl-3-nitro-
83-42-1: 1209: Benzene, 1-chloro-2-methyl-3-nitro-
83-44-3: 4091: Cholan-24-oic acid, 3,12-dihydroxy-, (3α,5β,12α)-
83-45-4: 11540: Stigmastan-3-ol, (3β,5α)-
83-46-5: 11542: Stigmast-5-en-3-ol, (3β)-
83-47-6: 11541: Stigmast-5-en-3-ol, (3β,24*S*)-
83-48-7: 11538: Stigmasta-5,22-dien-3-ol, (3β,22E)-
83-49-8: 4090: Cholan-24-oic acid, 3,6-dihydroxy-, (3α,5β,6α)-
83-53-4: 7792: Naphthalene, 1,4-dibromo-
83-54-5: 11312: 4(1H)-Quinolinone, 1-methyl-
83-56-7: 7827: 1,5-Naphthalenediol
83-60-3: 12046: Yohimban-16-carboxylic acid, 18-hydroxy-11,17-dimethoxy-, (3β,16β,17α,18β,20
83-66-9: 1460: Benzene, 1-(1,1-dimethylethyl)-2-methoxy-4-methyl-3,5-dinitro-
83-67-0: 10740: 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-
83-68-1: 7790: 1,4-Naphthalenediamine, 2-methyl-
83-72-7: 7849: 1,4-Naphthalenedione, 2-hydroxy-
83-73-8: 11298: 8-Quinolinol, 5,7-diiodo-
83-74-9: 7177: Ibogamine, 12-methoxy-
83-79-4: 2780: [1]Benzopyrano[3,4-b]furo[2,3-h][1]benzopyran-6(6aH)-one, 1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethen
83-81-8: 1323: 1,2-Benzenedicarboxamide, *N,N,N',N'*-tetraethyl-
83-88-5: 11327: Riboflavin
83-95-4: 6172: Furo[2,3-b]quinoline, 4,7,8-trimethoxy-
84-11-7: 9161: 9,10-Phenanthrenedione
84-15-1: 11578: 1,1':2',1"-Terphenyl
84-16-2: 9284: Phenol, 4,4'-(1,2-diethyl-1,2-ethanediyl)bis-, (*R*,S**)-
84-17-3: 9288: Phenol, 4,4'-(1,2-diethylidene-1,2-ethanediyl)bis-
84-26-4: 7324: Indolo[2',3':3,4]pyrido[2,1-b]quinazolin-5(7H)-one, 8,13-dihydro-
84-31-1: 4127: Cinchonan-9-one, 6'-methoxy-, (8α)-
84-52-6: 5014: 3'-Cytidylic acid
84-54-8: 409: 9,10-Anthracenedione, 2-methyl-
84-55-9: 10418: 1-Propanone, 3-(3-ethenyl-4-piperidinyl)-1-(6-methoxy-4-quinolinyl)-, (3*R-cis*)-
84-58-2: 4243: 1,4-Cyclohexadiene-1,2-dicarbonitrile, 4,5-dichloro-3,6-dioxo-
84-61-7: 1346: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
84-62-8: 1344: 1,2-Benzenedicarboxylic acid, diphenyl ester
84-65-1: 379: 9,10-Anthracenedione
84-66-2: 1348: 1,2-Benzenedicarboxylic acid, diethyl ester
84-68-4: 3029: [1,1'-Biphenyl]-4,4'-diamine, 2,2'-dichloro-
84-69-5: 1336: 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester
84-74-2: 1338: 1,2-Benzenedicarboxylic acid, dibutyl ester
84-79-7: 7851: 1,4-Naphthalenedione, 2-hydroxy-3-(3-methyl-2-butenyl)-
84-80-0: 7855: 1,4-Naphthalenedione, 2-methyl-3-(3,7,11,15-tetramethyl-2-hexadecenyl)-, [*R*-[*R*,R**-(*E*)]]-
84-86-6: 7956: 1-Naphthalenesulfonic acid, 4-amino-
84-87-7: 7961: 1-Naphthalenesulfonic acid, 4-hydroxy-
84-88-8: 11277: 5-Quinolinesulfonic acid, 8-hydroxy-
84-89-9: 7955: 1-Naphthalenesulfonic acid, 5-amino-
84-95-7: 7703: 1-Naphthalenamine, *N,N*-diethyl-
84-99-1: 2395: 2H,8H-Benzo[1,2-b:5,4-b']dipyran-2-one, 5-methoxy-8,8-dimethyl-
85-00-7: 5215: Diquat dibromide
85-01-8: 9150: Phenanthrene
85-02-9: 2434: Benzo[f]quinoline
85-23-4: 4253: 2,5-Cyclohexadiene-1,4-dione, 2,5-dihydroxy-3-methoxy-6-methyl-
85-29-0: 7593: Methanone, (2-chlorophenyl)(4-chlorophenyl)-
85-34-7: 942: Benzeneacetic acid, 2,3,6-trichloro-
85-38-1: 2644: Benzoic acid, 2-hydroxy-3-nitro-
85-41-6: 7352: 1H-Isoindole-1,3(2H)-dione
85-42-7: 7335: 1,3-Isobenzofurandione, hexahydro-
85-44-9: 7332: 1,3-Isobenzofurandione
85-46-1: 7965: 1-Naphthalenesulfonyl chloride
85-47-2: 7950: 1-Naphthalenesulfonic acid
85-55-2: 2681: Benzoic acid, 2-(4-methylbenzoyl)-
85-64-3: 9384: Phenol, 2-methoxy-5-[(1,2,3,4-tetrahydro-6,7-dimethoxy-2-methyl-1-isoquinolinyl)methyl]-, (±)-
85-66-5: 9183: Phenazinium, 1-hydroxy-5-methyl-, hydroxide, inner salt
85-73-4: 2723: Benzoic acid, 2-[[[4-[(2-thiazolylamino)sulfonyl]phenyl]amino]carbonyl]-
85-74-5: 7863: 1,7-Naphthalenedisulfonic acid, 4-amino-
85-75-6: 7862: 1,6-Naphthalenedisulfonic acid, 4-amino-
85-82-5: 8019: 2-Naphthalenol, 1-[(2,5-dimethylphenyl)azo]-
85-83-6: 8023: 2-Naphthalenol, 1-[[2-methyl-4-[(2-methylphenyl)azo]phenyl]azo]-
85-84-7: 7719: 2-Naphthalenamine, 1-(phenylazo)-
85-86-9: 8028: 2-Naphthalenol, 1-[[4-(phenylazo)phenyl]azo]-
85-90-5: 2830: 4H-1-Benzopyran-4-one, 3-methyl-
85-91-6: 2678: Benzoic acid, 2-(methylamino)-, methyl ester
85-95-0: 9289: Phenol, 4,4'-(1,2-diethyl-3-methyl-1,3-propanediyl)bis-
85-97-2: 3089: [1,1'-Biphenyl]-2-ol, 3-chloro-
85-98-3: 11986: Urea, *N,N'*-diethyl-*N,N'*-diphenyl-
86-00-0: 3082: 1,1'-Biphenyl, 2-nitro-
86-21-5: 10993: 2-Pyridinepropanamine, *N,N*-dimethyl-γ-phenyl-
86-26-0: 3078: 1,1'-Biphenyl, 2-methoxy-
86-28-2: 3978: 9H-Carbazole, 9-ethyl-
86-29-3: 967: Benzeneacetonitrile, α-phenyl-
86-30-6: 829: Benzenamine, *N*-nitroso-*N*-phenyl-
86-34-0: 11144: 2,5-Pyrrolidinedione, 1-methyl-3-phenyl-
86-48-6: 7764: 2-Naphthalenecarboxylic acid, 1-hydroxy-
86-50-0: 496: Azinphos-methyl
86-52-2: 7775: Naphthalene, 1-(chloromethyl)-
86-53-3: 7739: 1-Naphthalenecarbonitrile
86-55-5: 7756: 1-Naphthalenecarboxylic acid
86-56-6: 7706: 1-Naphthalenamine, *N,N*-dimethyl-

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