

THE
MERCK
INDEX
★
TWELFTH EDITION

THE MERCK INDEX

AN ENCYCLOPEDIA OF
CHEMICALS, DRUGS, AND BIOLOGICALS

TWELFTH EDITION

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Abbreviations and Selected Definitions

Please consult the Glossary (Misc. Tables Section) for additional definitions.

A	adenine; adenosine; absorbance (extinction)	A.S.T.M.	American Society for Testing Materials
Å	Angstrom units	as-, asym-	asymmetrical, unsymmetrical
AAT	α_1 -antitrypsin	at.	atomic
Ab	antibody	ATCC	American Type Culture Collection
abs	absolute; absorption	atm, atmos	atmosphere(s), atmospheric
abs config	absolute configuration	at. no.	atomic number
abstr	abstract	ATP	adenosine triphosphate
Abu	α -aminobutyric acid	ATPase	adenosine triphosphatase
Ac	acetyl $\text{CH}_3\text{CO}-$	at. wt.	atomic weight
acc	according	BAN	British Approved Name
ACE	angiotensin converting enzyme	B cell	bone marrow or bursa of Fabricius derived cell
Acetyl CoA	acetyl coenzyme A	BCG	Bacillus Calmette-Guerin
Ac_2O	acetic anhydride	Bé	Baumé (a specific gravity scale)
AcOEt	ethyl acetate	Beilstein	Beilstein's <i>Handbuch der Organischen Chemie</i>
AcOH	acetic acid	Belg. pat.	Belgian patent
ACP	acyl carrier protein	Ber.	<i>Chemische Berichte</i> (Berichte der Deutschen Chemischen Gesellschaft)
A.C.S.	American Chemical Society	BGG	bovine gamma globulin
ACTH	adrenocorticotrophic hormone	biol	biological
AcylSCoA	acyl coenzyme A	B.I.O.S.	British Intelligence Objectives Subcommittee
ADCC	antibody-dependent cellular cytotoxicity	BOC	<i>tert</i> -butoxycarbonyl
add(n)	adding, addition	B.O.D.	biochemical oxygen demand
Ade	adenine	boil.	boiling
ADH	alcohol dehydrogenase	bp	basepair; boiling point; boils at; boiling at Example: bp ₇₀ 48° means boils at 48°C if the pressure is 70 mm Hg
ADP	adenosine diphosphate	B.P.	British Pharmacopeia
AEC	(United States) Atomic Energy Commission	B.P.C.	British Pharmaceutical Codex
Ag	antigen, silver	Brit. pat.	British patent
AI	anaphylotoxin inhibitor	BRM	biological response modifier
AIDS	acquired immunodeficiency syndrome	BSA	bovine serum albumin
Ala	alanine	Btu	British thermal units
alc, alcohol	alcohol(ic); ethanol; ethyl alcohol	Bu	butyl
ALG	anti-lymphocyte globulin	Bz	benzoyl $\text{C}_6\text{H}_5\text{CO}-$
alk	alkali(ne)	BzH	benzaldehyde
$[\alpha]_D^{25}$	specific optical rotation at 25° C for D (sodium) line; absence of brackets indicates optical rotation of a liquid in a 1 decimeter cell, neat	BzOH	benzoic acid
ALS	anti-lymphocyte serum, amyotrophic lateral sclerosis	c	concentration by volume (g/100ml) after optical rotations only
a_M	molar absorptivity (concn in g-moles/l)	C	cytosine; cytidine; complement
amorph	amorphous	°C	Centigrade degrees; Celsius degrees
AMP	adenosine 5'-monophosphate (adenylic acid)	C_p	heat capacity (constant pressure)
cAMP	cyclic AMP	ca.	(circa) about
amps	ampules	C.A.	<i>Chemical Abstracts</i>
amt(s)	amount(s)	cal	calorie(s)
ANF	anti-nuclear factor; atrial natriuretic factor	calc(d)	calculate, calculated
anhydr	anhydrous	Can. pat	Canadian patent
anti	stereodescriptor, see Glossary	Cbz	carbobenzoxo
Ann.	<i>Justus Liebig's Annalen der Chemie</i>	cbc	complete blood count
APhA	American Pharmaceutical Association	cc	cubic centimeter(s) (milliliter)
approx	approximate(ly)	CCK	cholecystokinin
APT	alum precipitated toxoid	CD	circular dichroism
aq	aqueous	CDP	cytidine diphosphate
Ar	aryl	CEA	carcinoembryonic antigen
A.R.	analytical reagent	cf.	(confer) compare
ARC	AIDS related complex	CFA	complete Freund's adjuvant (same as FCA)
Archiv Exp. Pathol. Pharmacol.	<i>Naunyn Schmiedebergs Archiv für Experimentelle Pathologie und Pharmacologie</i>	CFT	complement fixation test
ArCO-	aromatic acyl radical	CHD	coronary heart disease
Arg	arginine	CHF	congestive heart failure
Asa	β -carboxyaspartic acid	chem	chemical
Asn	asparagine	Chem. Commun.	<i>Journal of the Chemical Society, Chemical Communications.</i>
Asp	aspartic acid	Ci	curie
assoc(d)	association; associated	C.I.	Colour Index (British)
		cis-	stereodescriptor, see Glossary
		cm	centimeter(s)

CM-cellulose
CMI
CML
CMP
CNS
CoA or CoASH
coll. vol.
compd
compn
Con A
conc(d)
concn
config
constit
contd
contg
CoQ
cor(r)
corresp
cp
C.P.
cpd
crit press
crit temp
crist
crystn
CSF
CTFA
CTP
Cys
Cyt
d
d-
Da
DEAE cellulose
dec, decomp
decompn
deg
deliquesce
 Δ (delta)
deriv
determin
DFP, DIFP, DIPF
Dha
Dhb
diff
dil(d), (n)
distln
dl-
DL-
dm
DMA
DMARD
DMF
DMSO
DNA
cDNA
mtDNA
DNAase
DNFB
DNP
Dopa
dp, DP
O-(carboxymethyl) cellulose
cell-mediated immunity
cell-mediated lymphocytotoxicity
cytidine 5'-monophosphate (cytidylic acid)
central nervous system
coenzyme A
collective volume
compound
composition
concanavalin A
concentrated
concentration
configuration
constituent
continued
containing
coenzyme Q (ubiquinone)
corrected
corresponding, corresponds
centipoise
chemically pure
compound
critical pressure
critical temperature
crystalline, crystals
crystallization
colony stimulating factor; cerebral spinal fluid
Cosmetic, Toiletary and Fragrance Assoc.
cytidine triphosphate
cysteine
cytosine
density; specific gravity (d_4^{20} specific gravity at 19° referred to water at 4°)
dextro(rotatory), the opposite of *l*
dextro (in configurational sense only), the opposite of *l*
daltons
O-(diethylaminoethyl)cellulose
decompose(s), decomposition
decomposition
degree
deliquescent
indicates the locant of the double bond
derivative
determination
diisopropyl fluorophosphate or diisopropyl phosphofluoridate
dihydroalanine
dehydrobutyrene,
 β -methyldehydroalanine
difference
dilute, diluted, dilution
distillation
racemic
optically inactive by external compensation as contrasted with *meso*-
decimeter(s)
dimethylacetamide
disease modifying antirheumatic drug
dimethylformamide
dimethylsulfoxide
deoxyribonucleic acid
complementary DNA
mitochondrial DNA
deoxyribonuclease
2,4-dinitro-1-fluorobenzene
2,4-dinitrophenyl or 2,4-dinitrophenol
dihydroxyphenylalanine
degree of polymerization (number of monomeric units in the polymer)

D.R.P.

ds
DTT
dyn
(E)-
 $E_{1\text{cm}}^{1\%}$
 E_M
EAA
EAC
EAE
EC
ECF-A
ECG
E.C. No.
ed.
ED
Ed(s).
EDTA
EEG
e.g.
EGF
eidem
EINECS
EKG
ELISA
emf
en
endo-
EPA
EPO
 ϵ (epsilon)
eq
equilib
equiv
esp
esu
Et
 η (eta)
et al.
etc.
 Et_2O
EtOH
Eur. pat. Appl.
ev
evac
evapn
exo-
expt(ly)
ext(d)
extern
°F
F-1-P
F-6-P
FA
FAB
FAD (FADH₂)
FCA
Fd
F.D.A.
FD & C

(Deutsches Reichs-Patent)-German patent
double stranded
dithiothreitol
dynes
entgegen, stereodescriptor, *see* Glossary
the absorbance of a solution containing one gram per 100 ml contained in a cell having an absorption path of one cm
molar extinction coefficient (concn in g-moles/l)
excitatory amino acid
erythrocyte coated by antibody and complement
experimental allergic encephalomyelitis
electron capture
eosinophil chemotactic factor of anaphylaxis
electrocardiogram
Enzyme Commission Number
edition
effective dose
editor(s)
ethylenediaminetetraacetic acid
electroencephalogram
(*exempli gratia*) for example
epidermal growth factor
the same (authors), plural of *idem*
European Inventory of Existing Chemical Substances
electrocardiogram
enzyme-linked immunosorbent assay
electromotive force
ethylenediamine (in formulas)
stereochemical descriptor, *see* Glossary
Environmental Protection Agency
erythropoietin; European Patent Office
molar extinction coefficient (concn in g-moles/l); dielectric constant
equation
equilibrium
equivalent
equivalent
especially
electrostatic units of electrical charge
ethyl C₂H₅-
viscosity
(*et alii*) and others
et cetera
ether
ethyl alcohol
European patent application
electron volt
evacuated
evaporation
stereochemical descriptor, *see* Glossary
experimental(ly)
extract, extracted
externally
Fahrenheit degrees; also Fourneau
fructose 1-phosphate
fructose 6-phosphate
fatty acid
fast atom bombardment
flavin adenine dinucleotide (reduced form)
Freund's complete adjuvant (same as CFA)
ferredoxin
Food and Drug Administration (U.S.A.)
Food, Drug and Cosmetic (U.S.A.)

FDNB
FDP
ff
FFA
FFC
FIA
FIAT
FMN (FMNH₂)
Fmoc
Fortschr. Chem. Org. Naturst.
fp
FP
FPLC
Fr. pat. Frdl.
Fru
FSH
FT
g
G
G-1-P
G-3-P
G-6-P
GABA
gal
Gal
GalNAc
 γ (gamma)
GC
GDH
GDP
gem-
geol
Ger. pat.
GH
GI
g/l
Gla
Glc
GLC
GlcA
GlcN
GlcNAc
GlcUA
Gln
Glu
GluA
Gly
Glycerol-3-P
Gmelin's
GMP
cGMP
GM-CSF
gov't
GP
GRF, GHRF
GSH
GSSG
GTP
GU
Gua

ichs-Patent)-German

ed

odescriptor, *see*

e of a solution
one gram per 100 ml
n a cell having an
path of one cm
ion coefficient (concn in

ino acid
ated by antibody and
it
allergic
nyelitis
ire
emotactic factor of
s
gram
mission Number

inetetraacetic acid
ialogram
ia) for example
owth factor
hors), plural of *idem*
entory of Existing
Substances
gram
d immunosorbent assay
force
ine (in formulas)
al descriptor, *see*

al Protection Agency
n; European Patent

ion coefficient (concn in
; dielectric constant

units of electrical charge

others

tent application

al descriptor, *see*

(ly)
cted

egrees; also Fourneau
osphate
osphate

mbardment
ie dinucleotide (reduced
nplete adjuvant (same as

ug Administration
and Cosmetic (U.S.A).

FDNB
FDP
ff
FFA
FFC
FIA

FIAT

FMN (FMNH₂)

Fmoc
*Fortschr. Chem.
Org. Naturst.*

fp
FP
FPLC
Fr. pat.
Frdl.

Fru
FSH
FT
g
G
G-1-P
G-3-P
G-6-P
GABA
gal
Gal
GalNAc
γ (gamma)
GC
GDH
GDP
gem-

geol
Ger. pat.
GH
GI
g/l
Gla
Glc
GLC
GlcA
GlcN
GlcNAc
GlcUA
Gln
Glu
GluA
Gly
Glycerol-3-P
Gmelin's

GMP

cGMP
GM-CSF

gov't
GP
GRF, GHRF
GSH
GSSG
GTP
GU
Gua

1-fluoro-2,4-dinitrobenzene
fructose 1,6-diphosphate
following
free fatty acid
free from chlorine
Freund's incomplete adjuvant (same
as ICFA)
Field Information Agency, Technical
(U.S. reports)
flavin mononucleotide (reduced
form); same as riboflavin
phosphate
9-fluorenylmethoxycarbonyl
*Fortschritte der Chemie Organischer
Naturstoffe* (Progress in the
Chemistry of Organic Natural
Products)
freezing point
flavoprotein
fast protein liquid chromatography
French patent
*P. Friedlander Fortschritte der Teer-
farbenfabrikation*, a collection of
patents
fructose
follicle-stimulating hormone
Fourier transform
gram(s)
guanine; guanosine
glucose 1-phosphate
glyceraldehyde 3-phosphate
glucose 6-phosphate
γ-aminobutyric acid
gallon(s)
galactose
N-acetyl-D-galactosamine
microgram(s)
gas chromatography
glutamate dehydrogenase
guanosine diphosphate
geminal, stereodescriptor *see*
Glossary

geological
German patent
growth hormone
gastrointestinal
grams per liter
γ-carboxyglutamic acid
glucose
gas-liquid chromatography
gluconic acid
glucosamine
N-acetyl-D-glucosamine
glucuronic acid
glutamine
glutamic acid
glucuronic acid
glycine
glycerol 3-phosphate
*Gmelin's Handbuch der
Anorganischen Chemie*, a
comprehensive German
encyclopedia of inorganic
chemistry
guanosine 5'-monophosphate
(guanylic acid)
cyclic GMP
granulocyte macrophage colony
stimulating factor
government
glycoprotein
growth hormone releasing factor
glutathione (reduced)
glutathione (oxidized)
guanosine triphosphate
genitourinary
guanine

GVH
habit.
Har
Hb
HbCO

HbO₂
HCG
Hcy
HDL
HeLa

HGG
HGH
His
HIV
Hiv
HLA
HMG-CoA

Houben

Houben Weyl

HPLC

hr
HSA
Hse
HSV
HT
HTLV

Hyl
Hyp
i-

I

Ia
IACR

IARC

IARC Monographs

ibid.

I.C.C.

ICFA

ICSH

IDDM
idem

IDP

i.e.

IEF

IF, IFN

i.g.

Ig

I.G. Farben

IGF-1

IL

Ile

i.m.

IMP

incl
incompat
INN

graft-versus-host
habitat
homoarginine
hemoglobin
carbon monoxide hemoglobin;
carboxyhemoglobin
oxyhemoglobin
human chorionic gonadotropin
homocysteine
high density lipoproteins
cells of the first continuously
cultured (human cervical)
carcinoma strain
human gamma globulin
human growth hormone
histidine
human immunodeficiency virus
α-hydroxyisovaline
human leukocyte antigen
3-hydroxy-3-methylglutaryl
coenzyme A
a German collection of medicinal
patents
*Houben-Weyl Methoden der
Organischen Chemie*, a German
collection of preparative methods
in organic chemistry
high performance (pressure, power)
liquid chromatography
hour
human serum albumin
homoserine
herpes simplex virus
hydroxytryptamine (serotonin)
human T lymphotropic virus *see also*
HTV
hydroxylysine
hydroxyproline
optically inactive by internal
compensation as *i*-inositol; archaic
for *meso*-
inosine
I-region antigen
International Association of Cancer
Registries
International Agency for Research on
Cancer
*IARC Monographs on the Evaluation
of Carcinogenic Risk of Chemicals
to Man*
(*ibidem*) at the same place
Interstate Commerce Commission
incomplete Freund's adjuvant (same
as FIA)
interstitial cell-stimulating hormone
(same as LH)
insulin dependent diabetes mellitus
the same (author); plural: *eidem*, the
same (authors)
inosine diphosphate
(*id est*) that is
Isoelectric focusing
interferon
intra gastric
immunoglobulin
*Interessengemeinschaft der
Farberindustrie, Aktiengesellschaft*—
the German dye trust
insulin-like growth factor 1
interleukin
isoleucine
intramuscular
inosine 5'-monophosphate (inosinic
acid)
including
incompatibility
International Nonproprietary Name

inorg inorganic
insol insoluble
intern internal
Intd International
i.p. intraperitoneal
IR infrared
Ir genes immune response genes
ISO Internal Organization for
Standardization
isolation
ITP inosine triphosphate; idiopathic
thrombocytopenic purpura
international unit
I.U. International Union of Chemistry
I.U.C. International Union of Pure and
I.U.P.A.C. Applied Chemistry
i.v. intravenous
Japan. Kokai Japanese patent (unexamined)
Japan. pat. Japanese patent
K dissociation constant; equilibrium
constant
°K degrees Kelvin
Kb kilobase
kcal kilocalories(s)
K cell killer cell
kg kilogram(s)
αKG α-ketoglutarate
KLH keyhole limpet hemocyanin
KPA kidney plasminogen activator
l liter
l- *levo*(rotatory), the opposite of *d*
L- *levo* (in configurational sense only),
the opposite of *D*
Lac lactose
LAD lymphocyte-activating determinant
λ (lambda) wavelength
LAMMA laser microprobe mass analysis
LATS long acting thyroid stimulator
lb pound(s)
LC lethal concentration; liquid
chromatography
LC₅₀ median lethal concentration, the
concn of a chemical that is
estimated to be fatal to 50% of the
organisms tested
LCM lymphocyte choriomeningitis
LD lethal dose
LD₅₀ median lethal dose, the quantity of a
chemical that is estimated to be
fatal to 50% of the organisms
tested
LDH lactate dehydrogenase
LDL low density lipoproteins
Leu leucine
LH luteinizing hormone (same as ICSH)
ln natural logarithm
loc. cit. (*loco citato*) in the place cited
log logarithm (common)
l.o.i. limit of impurities
LPS lipopolysaccharide
Lys lysine
m meter; given after mass number
signifies metastable isomer
m- *meta* chemical locant for ring
substituents
M molar (concentration)
Mab, mAb monoclonal antibody
MAC maximum allowable concentration
MAF macrophage activating factor
MAO monoamine oxidase
MAOI monoamine oxidase inhibitor
mass spec mass spectrometry
max maximum, maxima
Mb myoglobin
MbO₂ oxy-myoglobin
M.C.A. Manufacturing Chemists Association
(U.S.A.)

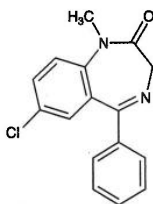
mcg microgram
mCi millicurie
MD molecular rotation $\frac{[\alpha]_D \times \text{mol wt}}{100}$
MDH malate dehydrogenase
Me methyl CH₃—
Me₂CO— acetone
MeOH methyl alcohol
Mellor's *Mellor's Comprehensive Treatise on
Inorganic and Theoretical
Chemistry*
mEq milli-equivalent (0.001 of an
equivalent)
Met methionine
fMet *N*-formylmethionine
MetHb methemoglobin
meV millielectron volts
mfg, manuf manufacturing
mfr manufacture
mg milligram
MHC major histocompatibility complex
mCi microcurie
mg microgram
microcryst microcrystalline
MIF migration inhibition factor
min minimum; minute(s)
MIS Mullerian inhibiting substance
misc miscible
mixt mixture
ml milliliter (cubic centimeter)
MLD minimum lethal dose
MLR mixed lymphocyte reaction
mm millimeter
mμ millimicron(s), nm
mol wt molecular weight
Monatsh. *Monatshefte für Chemie*
mOsm milliosmolar
mp melting point; melts, melting at,
when followed by a figure
denoting temperature
M, relative molecular mass
MRI magnetic resonance imaging
ms- *meso*- (internally compensated)
MS mass spectrometry
MSH melanocyte-stimulating hormone
(melanotropin)
n index of refraction (n_D^{20} for 20° and
sodium light); normal, as *n*-propyl
N normal (equivalents per liter, as
applied to concentration); nitrogen
(as in *N*-methylpyridine)
Nacneu *N*-acetylneuraminic acid
NAD⁺ (NADH) nicotinamide adenine dinucleotide
(reduced form)
NADP⁺ (NADPH) nicotinamide adenine dinucleotide
phosphate (reduced form)
NANSAIDS nonaspirin nonsteroidal anti-
inflammatory drugs
NBS National Bureau of Standards
NCTC *National Collection of Type Cultures*
NDP nucleoside 5'-phosphate
Neth. pat. Appl. Netherlands patent application
N.F. *National Formulary*
ng nanogram (10⁻⁹ grams)
NGF nerve growth factor
NIDDM Non-insulin dependent diabetes
mellitus
NIOSH National Institute for Occupational
Safety and Health
nm nanometer
NMN⁺ (NMNH) nicotinamide mononucleotide
(reduced form)
NMP nucleoside 5'-monophosphate
NMR nuclear magnetic resonance
N.N.D. *New and Nonofficial Drugs*
(Lippincott, 1959-1964)

N.N.R. A
no. n
nor- c
NRDC N
NSAID(s) n
NSC N
NTP n
o- o
O d
OA o
OAA o
OD o
op. cit. (c
org o
OSHA O
Osm o
oz. o
P, p c
P, PP p
P- p
Pi in
Pa p
PABA p-
PAF pl
PAGE p
passim h
pat. p
PB report P
PCA p
PCT P
PEP p
PET p
petr, petrol pe
PFC pl
3PG 3-
PG pr
PGA pr
PGP pt
pH 3-
ac
PHA ph
Phe ph
physiol ph
pK lo
PKU ph
PMN po
PPi in
ppm pa
ppt(g) pr
pptd pr
PQ pli
Pr pr
prepd pr
prepn pr
press. pr
Pro pr
PRPP 5-
ψ (psi) p
pt ps
PTH po
Q pa
q-q.v. co
q.v. (q
r (q
r- r
rac

$x)_D \times \text{mol wt}$	N.N.R.	<i>New and Nonofficial Remedies</i> (Lippincott, 1933-1958)	R	alkyl, univalent hydrocarbon radical (or hydrogen)
100	no.	number	(R)-	<i>rectus</i> (right), stereodescriptor <i>see</i> <i>Glossary</i>
se	nor-	chemical nomenclature descriptor, <i>see Glossary</i>	RAST	radioallergosorbent test
	NRDC	National Research Development Corporation	rbc	red blood cell; red blood count
	NSAID(s)	nonsteroidal anti-inflammatory drugs	RCO-	aliphatic acyl radical
	NSC	National Service Center	recryst(n)	recrystallize, recrystallization
<i>isive Treatise on</i>	NTP	nucleoside 5'-triphosphate; National Toxicology Program (U.S.)	ref	reference
<i>eoretical</i>		<i>ortho</i> chemical locant for ring substituents	rep [REP]	"roentgen equivalent physical" means a dose of ionizing radiation capable of producing energy absorption of 93 ergs per gram of tissue
01 of an	O-	denoting attachment to oxygen, as in O- acetylhydroxylamine	resp	respectively
	O	ovalbumin	R _f or R _F	(in paper chromatography) ratio of movement of the band to the front of the solvent
	OA	oxaloacetate	RIA	radioimmunoassay
	OAA	optical density	Rib	D-ribose
	OD	(<i>opere citato</i>) in the work cited	RIST	radioimmunosorbent test
	op. cit.	organic	RNA	ribonucleic acid
	org	Occupational Safety and Health Act	hnRNA	heterogeneous nuclear RNA
bility complex	OSHA	ounce(s)	mRNA	messenger RNA
	OsM	concentration by weight (after optical rotations only)	nRNA	nuclear RNA
	oz.	page(s)	rRNA	ribosomal RNA
1 factor	P, p	<i>para</i> chemical locant for ring substituents	snRNA	small nuclear RNA
i)	p, pp	inorganic phosphate	tRNA	transfer (soluble) RNA
g substance	p-	pascal	RNase	ribonuclease
	Pi	<i>p</i> -aminobenzoic acid	RTECS	<i>Registry of Toxic Effects of Chemical Substances</i>
timeter)	Pa	platelet-activating factor	s-	symmetrical
se	PABA	polyacrylamide gel electrophoresis	S	denoting attachment to sulfur as in S-methylcysteine
reaction	PAF	here and there, scattered	(S)-	<i>sinister</i> (left), stereodescriptor <i>see</i> <i>Glossary</i>
	PAGE	patent	S.A.E.	Society of Automotive Engineers
	passim	Publication Board Report (United States Department of Commerce, Scientific and Industrial Reports)	SAM	S-adenosylmethionine
hemie	pat.	passive cutaneous anaphylaxis	sapon(if)	saponification
	PB report	Patent Co-operation Treaty	Sar	sarcosine
ts, melting at,		phosphoenolpyruvate	satd	saturated
oy a figure	PCA	positron emission tomography	s.c.	subcutaneous
ature	PCT	petroleum	SDS	sodium dodecyl sulfate
mass	PEP	plaque-forming cell	sec	second(s)
e imaging	PET	3-phosphoglycerate	sec-	secondary
compensated)	petr.	prostaglandin	sepn	separation
ating hormone	PFC	pteroylglutamic acid (folic acid)	Ser	serine
	3PG	3-phosphoglyceroyl phosphate	SI	International System of Units
1 (n_D^{20} for 20° and	PG	acid-base scale; log of reciprocal of hydrogen ion concentration	SLE	systemic lupus erythematosus
ormal, as <i>n</i> -propyl	PGA	phytohemagglutinin	SNRI	serotonin-noradrenaline reuptake inhibitor
ts per liter, as	PGP	phenylalanine		soluble; solubility
entration); nitrogen	pH	physiological	sol; soly	solidifies, solidification
pyridine)	PHA	log of the reciprocal of the dissociation constant, 1/log K	solidif	solution
ic acid	Phe	phenylketonuria	soln	species; specific
ine dinucleotide	physiol	polymorphonuclear leukocyte	sp.	spectroscopy
	pK	inorganic pyrophosphate	spec	single photon emission computed tomography
ine dinucleotide	PKU	parts per million	SPECT	specific gravity
aced form)	PMN	precipitate, precipitating	sp gr	species (plural)
roidal anti-	PPi	precipitated	spp.	square
rugs	ppm	plastoquinone	sq	(<i>sequentia</i>) and following
of Standards	ppt(g)	propyl (normal)	sqq	sheep red blood cells
on of Type Cultures	pptd	prepared	SRBC	slow reacting substance of anaphylaxis
sphate	PQ	preparation	SRS-A	single stranded
it application	Pr	pressure	ss	subacute sclerosing panencephalitis
try	prep	proline	SSPE	selective serotonin reuptake inhibitor
grams)	press.	5-phosphoribosyl 1-pyrophosphate	SSRI	standard temperature and pressure
tor	Pro	pseudo	S.T.P.	sublimes
ndent diabetes	PRPP	point	subl	supplement
for Occupational	ψ (psi)	parathyroid hormone	suppl	symmetrical
alth	pt	coenzyme Q (ubiquinone)	sym-	stereochemical descriptor <i>see</i> <i>Glossary</i>
nonnucleotide	PTH	(<i>quae vide</i>) which see, plural	syn-	thymine; thymidine
)	Q	(<i>quod vide</i>) which see	T	half-life
nophosphate	q.q.v.	"roentgen" unit of radiation	t _{1/2}	tablet(s)
resonance	q.v.	racemic	tabl	
cial Drugs	r			
359-1964)	r-			

TB, tb	tuberculosis	U.S.D.	<i>United States Dispensatory</i>
TCA	trichloroacetic acid; tricarboxylic acid	U.S.D.A.	United States Department of Agriculture
T cell	thymus derived cell	U.S.P.	<i>United States Pharmacopeia</i>
TDL	thoracic duct lymphocyte	U.S. pat.	United States patent
TDP	thymidine diphosphate	UTP	uridine triphosphate
TEAE cellulose	<i>O</i> -(triethylaminoethyl)-cellulose	uv	ultraviolet
tech	technical	v	volt(s)
temp	temperature	v-	vicinal (adjacent)
<i>tert</i> -	tertiary	Val	valine
TH	thyrotropic hormone	var	variety
THF	tetrahydrofuran	viz.	(<i>videlicet</i>) that is to say; namely
THFA	tetrahydrofolic acid	VLDL	very low density lipoproteins
Thr	threonine	vol	volume
Thy	thymine	vs	versus
TLC	thin-layer chromatography	v/v	percent "volume in volume"
TMP	thymidine 5'-monophosphate		expresses the number of milliliters of an active constituent in 100 milliliters of solution
TMV	tobacco mosaic virus	wbc	white blood cell; white blood count
TNF	tumor necrosis factor	WHO	World Health Organization
TNP	trinitrophenyl	wks	weeks
TPA	tissue plasminogen activator	wt	weight
TPP, ThPP	thiamine pyrophosphate	w/v	percent "weight in volume"
<i>trans</i> -	stereodescriptor <i>see Glossary</i>		expresses the number of grams of an active constituent in 100 milliliters of solution, and is used regardless of whether water or another liquid is the solvent
Tris	tris(hydroxymethyl)aminomethane; 2-amino-2-hydroxymethylpropane-1,3-diol	w/w	percent "weight in weight"
Trp	tryptophan		expresses the number of grams of an active constituent in 100 grams of solution or mixture
TSH	thyroid-stimulating hormone	XMP	xanthosine monophosphate
TSTA	tumor-specific transplantation antigens	yr(s)	year(s)
TTP, dTTP	thymidine triphosphate	Z	carbobenzoxy
Tyr	tyrosine	(Z)-	<i>zusammen</i> stereodescriptor <i>see Glossary</i>
U	uracil or uridine	Z. <i>Physiol.</i>	<i>Hoppe-Seyler's Zeitschrift für Physiologische Chemie</i>
UDP	uridine diphosphate	~	approximately
UDP-gal	uridine diphosphogalactose	≈	approximately equal
UDP-glc	uridine diphosphoglucose	>	greater than
U.K.	United Kingdom	<	less than
UMP	uridine 5'-monophosphate (uridylic acid)		
uncor(r)	uncorrected		
<i>uns</i> -, <i>unsym</i> -	unsymmetrical, asymmetrical		
Ura	uracil		
U.S.A.E.C.	United States Atomic Energy Commission		
USAN	United States Adopted Names		

3042. Diazepam. 7-Chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one; 7-chloro-1-methyl-5-phenyl-3H-1,4-benzodiazepin-2(1H)-one; methyl diazepam; diazepam; LA-III; Ro-5-2807; Wy-3467; NSC-77518; Apaurin; Atensine; Atilen; Bialzepam; Calmpose; Cereglart; Dialar; Diazemuls; Dipam; Eridan; Eurosan; Evacalm; Faustan; Gewacalm; Horizol; Lamra; Lembrol; Levium; Mandrozep; Neurolytril; Noan; Novazam; Paccum; Pacitrin; Paxate; Paxel (obsolete); Pro-Pam; Q-Pam; Relanium; Sedapam; Seduxen; Servizepam; Setonil; Solis; Stesolid; Tranquase; Tranquo-Puren; Tranquo-Tablinen; Unisedil; Valaxona; Valiquid; Valium; Valrelease; Vival; Vivol. $C_{16}H_{13}ClN_2O$; mol wt 284.74. C 67.49%, H 4.60%, Cl 12.45%, N 9.84%, O 5.62%. Prepn: Sternbach, Reeder, *J. Org. Chem.* 26, 4936 (1961); Reeder, Sternbach, U.S. pat. 3,371,085 (1968 to Hoffmann-La Roche); prep but not claimed: eidem, U.S. pats. 3,109,843 and 3,136,815 (1963, 1964 to Hoffmann-La Roche); M. Gates, *J. Org. Chem.* 45, 1675 (1980); M. Ishikura *et al.*, *ibid.* 47, 2456 (1982). Purification: Chase, U.S. pat. 3,102,116 (1963 to Hoffmann-La Roche). Pharmacology: Hudson, Wolpert, *Arch. Int. Pharmacodyn. Ther.* 186, 388 (1970). Metabolism: Randall *et al.*, *Curr. Ther. Res. Clin. Exp.* 7, 590 (1965); Van der Kleijn, *Ann. N.Y. Acad. Sci.* 179, 115 (1971). Toxicity: E. I. Goldenthal, *Toxicol. Appl. Pharmacol.* 18, 185 (1971). Binding study in rat brain: R. F. Squires, C. Braestrup, *Nature* 266, 732 (1977). Comprehensive description: A. MacDonald *et al.*, *Anal. Profiles Drug Subs.* 1, 79-99 (1972). Clinical pharmacokinetics: M. Mandelli *et al.*, *Clin. Pharmacokinet.* 3, 72 (1978).

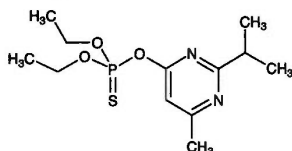


Plates from acetone + petr ether, mp 125-126°. pK_a 3.4. Sol in chloroform, DMF, benzene, acetone, alc; slightly sol in water. LD_{50} orally in rats: 710 mg/kg (Goldenthal).

Note: This is a controlled substance (depressant) listed in the U.S. Code of Federal Regulations, Title 21 Part 1308.14 (1995).

THERAP CAT: Anxiolytic; muscle relaxant (skeletal).

3043. Diazinon. Phosphorothioic acid *O*,*O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester; thiophosphoric acid 2-isopropyl-4-methyl-6-pyrimidyl diethyl ester; *O*,*O*-diethyl *O*-2-isopropyl-4-methyl-6-pyrimidyl thiophosphate; diethyl 2-isopropyl-4-methyl-6-pyrimidyl thionophosphate; dimpylate; G-24480; Antigal; Basudin; Diazol; D-z-n; Garden Tox; HelfaCat; HelfaDog; Neocidol; Parasetix; Sarolex; Spectracide; Taberdog; Tabergat. $C_{12}H_{19}N_3O_2PS$; mol wt 304.35. C 47.36%, H 6.95%, N 9.20%, O 15.77%, P 10.18%, S 10.54%. Prepn: Gysin, Margot, U.S. pat. 2,754,243 (1956 to Geigy). Insecticidal properties: Gasser, *Z. Naturforsch.* 8b, 225 (1953). Toxicity data: T. B. Gaines, *Toxicol. Appl. Pharmacol.* 14, 515 (1969).



Liquid. Faint ester-like odor. d_4^{20} 1.116-1.118. $bp_{0.002}$ 83-84°. n_D^{20} 1.4978-1.4981. Vapor pressure at 20°: 1.4×10^{-4} ; at 40°: 1.1×10^{-3} (~5 times vapor pressure of parathion). Volatility at 20°: 2.4 mg/m³; at 40°: 17.6 mg/m³. Decomposes above 120°. Soly in water at 20°: 0.004%. Miscible with alcohol, ether, petr ether, cyclohexane, benzene, and

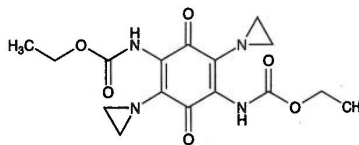
similar hydrocarbons. More stable in alkaline formulations, then when at neutral or acid pH. LD_{50} in male, female rats (mg/kg): 250, 285 orally (Gaines).

Caution: Cholinesterase inhibitor. *Clinical Toxicology of Commercial Products*, R. E. Gosselin *et al.*, Eds. (Williams & Wilkins, Baltimore, 5th ed., 1984) Section II, p 294.

USE: Insecticide.

THERAP CAT (VET): Ectoparasiticide.

3044. Diaziquone. [2,5-Bis(1-aziridinyl)-3,6-dioxo-1,4-cyclohexadiene-1,4-diyl]biscarbamic acid diethyl ester; 2,5-bis(1-aziridinyl)-3,6-dioxo-1,4-cyclohexadiene-1,4-dicarbamate diethyl ester; 2,5-diaziridinyl-3,6-bis(ethoxycarbonylamino)-1,4-benzoquinone; aziridinylbenzoquinone; AZQ; CI-904; NSC-182986. $C_{16}H_{20}N_4O_6$; mol wt 364.36. C 52.74%, H 5.53%, N 15.38%, O 26.35%. Quinone-containing lipophilic alkylating agent. Prepn as intermediate in dyestuffs: S. Petersen *et al.*, U.S. pat. 2,913,453 (1959 to Schenley Ind.). Synthesis and antitumor activity: A. H. Khan, J. S. Driscoll, *J. Med. Chem.* 19, 313 (1976); J. S. Driscoll *et al.*, U.S. pat. 4,146,622 (1979 to U.S. Gov't). *In vivo* antitumor studies: J. S. Driscoll *et al.*, *J. Pharm. Sci.* 68, 185 (1979). Intracerebral penetration and tissue distribution in humans: N. Savaraj *et al.*, *J. Neuro-Oncol.* 1, 15 (1983). LC determ: B. A. Allen *et al.*, *J. Chromatog.* 222, 146 (1981). Pharmacokinetics: S. Zimm *et al.*, *Cancer Res.* 44, 1698 (1984). Clinical studies in treatment of CNS neoplasms: R. T. Eagan *et al.*, *J. Neuro-Oncol.* 5, 309 (1987); E. Tapazoglou *et al.*, *Am. J. Clin. Oncol.* 11, 474 (1988). Review: J. F. Bender *et al.*, *Invest. New Drugs* 1, 71-84 (1983).



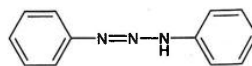
Orange needles from ethanol, mp 230° (dec); also reported as yellowish-brown crystals from ethanol decomposing at temperatures above 250° (Petersen). uv max (methanol): 340 nm ($\log \epsilon$ 4.17). Soly in water: 0.5 mg/ml. LD_{50} in mice (mg/m²): 30.9 i.v. (Bender).

THERAP CAT: Antineoplastic.

3045. Diazoacetic Ester. Ethyl diazoacetate; ethyl diazoethanoate. $C_4H_7N_2O_2$; mol wt 114.10. C 42.11%, H 5.30%, N 24.55%, O 28.04%. $-N=N+=CHCOOCH_2CH_3$. Prepd by the action of sodium nitrite on glycine ethyl ester hydrochloride: Curtius *J. Prakt. Chem.* [2] 38, 396 (1888); Silberrad, *J. Chem. Soc.* 81, 600 (1902); Womack, Nelson, *Org. Syn.* 24, 56 (1944).

Yellow oil. Pungent odor. Very volatile. Explosive. Distillation, even under reduced pressure, is dangerous. mp -22°. d_4^{16} 1.0852. bp_3 42°; bp_{12} 45°; bp_{28} 85-86°; bp_{76} 140-141°. n_D^{16} 1.4588. Slightly sol in water. Neutral reaction. Volatile with steam, ether, and benzene vapors. Miscible with alcohol, benzene, ligroin, ether. Explodes on contact with concd H_2SO_4 .

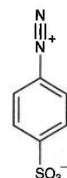
3046. Diazoaminobenzene. 1,3-Diphenyl-1-triazene; anilinoazobenzene; benzeneazoaniline. $C_{12}H_{11}N_3$; mol wt 197.24. C 73.07%, H 5.62%, N 21.30%. Made by diazotizing aniline dissolved in HCl with $NaNO_2$ and then adding a concd soln of sodium acetate: Hartman, Dickey, *Org. Syn. coll. vol. II*, 163 (1943).



Golden-yellow, small crystals. mp 98°; explodes when heated to 150°. Insol in water; freely sol in benzene, ether, hot alc.

3047. p-Diazobenzenesulfonic Acid. 4-Sulfobenzenediazonium inner salt; sulfanilic acid diazide. $C_6H_5N_3O_3S$; mol wt 184.18. C 39.13%, H 2.19%, N 15.21%, O 26.06%. S. Prepn by diazotization of sulfanilic acid and struc-

ture: Whetsel *et al.*, *J. Am. Chem. Soc.* 76, 767 (1954); Bugg *et al.*, *Acta Cryst.* 17, 767 (1961).



White or slightly red crystals by heat, a blow, or on rubbing. Slightly sol in cold water, alc, alkalis, HCl.

USE: As reagent for phenol, aldehydes, and albumin; also dyes.

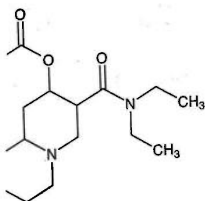
3048. Diazomethane. Az 42.04. C 28.57%, H 4.80%. Prepd from chloroform and potassium hydroxide: Staud (1912); McManus *et al.*, *J. Org. Chem.* 19, 100 (1954). These methane. The following pro diazomethane. From *N*-nitro methyl ketone in ether and sodium isopropoxide or from reaction with sodium cyclohexylmethylurea in ether: Arndt, (1943), or of nitrosomethylurea Ber. 27, 1888 (1894); 28, 855 Ber. 61, 1845 (1928). In the prep most simply by the commercially available *N*-methyl-*N*-nitrosomethylurea: McKay, *J. Am. Chem. Soc.* 68, 683 (1946). Chemistry (Reinhold, New York): 1955.

Very toxic yellow gas. Explodes on contact with glass. Avoid vapor. mp -145°; bp 36°; bp₁₂ 45°; bp₂₈ 85-86°; bp₇₆ 140-141°. n_D^{16} 1.4588. Slightly sol in water. Neutral reaction. Volatile with steam, ether, and benzene vapors. Miscible with alcohol, benzene, ligroin, ether. Explodes on contact with concd H_2SO_4 .

USE: Powerful methylating agent as carboxylic acids, phenols, etc. (1938); Eistert, *Z. Angew. Chem.* 1948. See Spangler in *Newer Methods in Organic Chemistry* (New York, 1948) Reagents vol. 2 (John Wiley, N

Freely sol in water, alc. Practically soln has a pH of 4.5 to 5.5. uv

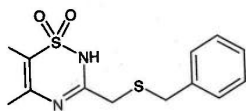
2-(Acetoxy)-N,N-diethyl-1,3,4-ethoxy-2H-benzof[quinolizine-3,3,4,6,7,11b-hexahydro-2-hydroxy-quinolizine-3-carboxamide acetylcarboxamido]-9,10-dimethyl-11bH-benzopyridocoline; 2-hydro-dimethoxy-1,2,3,4,6,7-hexahydroacetate; BZQ; NSC-64375; Promicon; Quantril. $C_{27}H_{32}N_4O_6$; 65.32%, H 7.97%, N 6.93%, O 19.78%. U.S. pat. 3,053,845 (1962) to Crabtree et al., *J. Am. Med. Assoc.* 186, 100 (1962); *Arch. Int. Pharmacodyn.* 186, 100 (1962). Metabolic studies: Koe, 635 (1964); Wiseman et al., *Biochem. Pharmacol.* 18, 185 (1971).



opyl ether, mp 130-131.5°. LD₅₀ kg; i.p. in mice: 376 mg/kg (Gol-

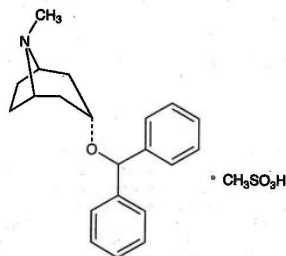
hotic, antiemetic.

6-Chloro-3-[(phenylmethyl)thio]thiadiazine-7-sulfonamide 1,1-diox-yl]-6-chloro-2H-1,2,4-benzothiadiazine-1,1-dioxide; 3-[(benzylthio)methyl]-6-benzo-1,2,4-thiadiazine 1,1-dioxide; -benzylthiomethyl-2H-1,2,4-benzothiadiazine; Aquatag; Dihydrex; la; Exosalt; Fovane; Freuril; Hy-lua; Urese. $C_{19}H_{14}ClN_4O_4S_2$; mol wt 444.244 (1962, 1969 both to Pfizer). S. Y. P'an et al., *J. Pharmacol.* 960.



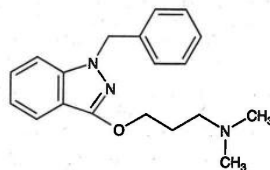
one, mp 231-232° (U.S. patent); also 239° (P'an). Bitter taste. Practically in alkaline solns. LD₅₀ in mice, rats 10000 orally; 410, 422 i.v. (P'an). tic, antihypertensive.

12 Mesylate. 3-(Diphenylmethoxy)-8,1,2,10-octane methanesulfonate; 3α-(di-5αH-tropine methanesulfonate; benz-nate; tropine benzohydryl ether meth-in; Cogentinol; Cobrentin methanesul-; mol wt 403.54. C 65.48%, H 7.24%, S 7.95%. Prep'd by the action of di-on tropine: Phillips, U.S. pat. 2,595, & Co.). Crystal structure: P. G. Jones *et al.* B34, 3125 (1978).



Crystals from acetone + ether, mp 143°. uv max: 259 nm ($E_{1\%}^{1cm} = 437$). Soluble in water. pH about 6. THERAP CAT: Anticholinergic.

1157. Benzylamine. N,N-Dimethyl-3-[[1-(phenylmethyl)-1H-indazol-3-yl]oxy]-1-propanamine; 1-benzyl-3-[[3-(dimethylamino)propoxy]-1H-indazole; 1-benzyl-1H-indazol-3-yl 3-(dimethylamino)propyl ether; benzindamine. $C_{19}H_{23}N_3O$; mol wt 309.41. C 73.76%, H 7.49%, N 13.58%, O 5.17%. Prep'n: Fr. pat. 1,382,855; Palazzo, U.S. pat. 3,318,905 (1964, 1967 both to Angelini Francesco); Palazzo et al., *J. Med. Chem.* 9, 38 (1966). Pharmacology: Lisciani et al., *Eur. J. Pharmacol.* 3, 157 (1968). Metabolism: Catanesi et al., *Arzneimittelforsch.* 16, 1354 (1966); Kataoka et al., *Chem. Pharm. Bull.* 19, 1511 (1971). Toxicology: B. Silvestrini et al., *Toxicol. Appl. Pharmacol.* 10, 148 (1967). Series of articles on pharmacology: *Arzneimittelforsch.* 37, 587-646 (1987).



bp_{0.05} 160°.

Hydrochloride, $C_7H_9N_2O.HCl$, Afloben, Andolex, Benalgin, Benzyrin, Diffiam, Dorinamin, Enzamin, Imotryl, Ririlim, Riripen, Salyzorin, Saniflor, Tamas, Tantum, Verax. Crystals, mp 160°. uv max: 306 nm ($E_{1\%}^{1cm} = 160$). Very sol in water; rather sol in ethanol, chloroform, n-butanol. LD₅₀ in mice, rats (mg/kg): 110, 100 i.p.; 515, 1050 orally (Silvestrini).

THERAP CAT: Analgesic; anti-inflammatory; antipyretic. THERAP CAT (VET): Anti-inflammatory.

1158. Benzyl Acetate. Acetic acid phenylmethyl ester; acetic acid benzyl ester. $C_9H_{10}O_2$; mol wt 150.18. C 71.98%, H 6.71%, O 21.31%. $C_6H_5CH_2COOCH_3$. Occurs in a number of plants, particularly jasmine: S. Arctander, *Perfume and Flavor Materials of Natural Origin* (Elizabeth, N.J., 1960) pp 313-314. Prep'd from benzyl chloride, acetic acid or sodium acetate and triethylamine: Merker, Scott, *J. Org. Chem.* 26, 5180 (1961); Dennis et al., *Ind. Eng. Chem., Prod. Res. Develop.* 6, 193 (1967). Toxicity study: P. M. Jenner et al., *Food Cosmet. Toxicol.* 2, 327 (1964).

Liquid; pear-like odor. bp 213°, bp₁₀₂ 134°. mp -51°. d_4^{25} 1.050. n_D^{20} 1.5232, n_D^{25} 1.4998. Flash pt, closed cup: 216° F (102° C). Practically insol in water. Misc with alcohol, ether. LD₅₀ orally in rats: 2490 mg/kg (Jenner).

Caution: If ingested can cause G.I. irritation with vomiting and diarrhea. Also irritating to skin, eyes, respiratory tract.

USE: In perfumery, solvent for cellulose acetate and nitrate.

1159. Benzyl Alcohol. Benzenemethanol; phenylcarbinol; phenylmethanol; α-hydroxytoluene. C_7H_8O ; mol wt 108.14. C 77.75%, H 7.46%, O 14.80%. $C_6H_5CH_2OH$. Constituent of jasmine, hyacinth, ylang-ylang oils, Peru and Tolu balsams, storax, where it occurs in ester form also.

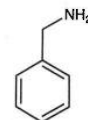
Originally prep'd by the Cannizzaro reaction from benzaldehyde + KOH: Cannizzaro, *Ann.* 88, 129 (1853); cf. Hickinbottom, *Reactions of Organic Compds.* (Longmans, London, 3rd ed., 1957) p 251; A. I. Vogel, *Practical Organic Chemistry* (Longmans, London, 3rd ed., 1959) p 711; Gattermann-Wieland, *Praxis des organischen Chemikers* (de Gruyter, Berlin, 40th ed., 1961) p 193. Produced on a large scale by the action of sodium or potassium carbonate on benzyl chloride: Ger. pat. 484,662; *Chem. Zentr.* 1930, I, 1052; *Frdl.* 16, 426; cf. Kirk-Othmer *Encyclopedia of Chemical Technology* vol. 3 (Interscience, New York, 1964) pp 442-449. Toxicity: Smyth et al., *Arch. Ind. Hyg. Occup. Med.* 4, 119 (1951).

Liquid. Faint aromatic odor. Sharp burning taste. d_4^{20} 1.04535; d_4^{25} 1.04156. mp -15.19°. bp₇₆₀ 204.7°; bp₄₀₀ 183.0°; bp₂₀₀ 160.0°; bp₁₀₀ 141.7°; bp₆₀ 129.3°; bp₃₀ 119.8°; bp₂₀ 105.8°; bp₁₀ 92.6°; bp₅ 80.8°; bp_{1.0} 58.0°. n_D^{20} 1.54035; n_D^{25} 1.53837. Dreisbach, *Martin, Ind. Eng. Chem.* 41, 2875 (1941). Absorption spectrum: Brode, *J. Phys. Chem.* 30, 61 (1926). Vapor density 3.72 (air = 1.00). Flash pt, closed cup 213°F, open cup 220°F. Autoignition temp 817°F. One gram dissolves in about 25 ml water. One volume dissolves in 1.5 vols of 50% ethyl alcohol. Misc with abs and 94% alcohol, ether, chloroform. LD₅₀ orally in rats: 3.1 g/kg (Smyth).

USE: Manuf other benzyl compds. Pharmaceutical aid (antimicrobial). Solvent for gelatin, casein (when hot), solvent for cellulose acetate, shellac. Used in perfumery and in flavoring (mostly in form of its aliphatic esters). In microscopy as embedding material.

THERAP CAT (VET): Has been used for relief from pruritis.

1160. Benzylamine. Benzenemethanamine; aminotoluene; phenylmethylaniline; moringine. C_7H_9N ; mol wt 107.16. C 78.46%, H 8.47%, N 13.07%. Prep'n from benzyl-chloride and ammonia: Mason, *J. Chem. Soc.* 63, 1311 (1893); by redn of benzonitrile: Carothers, Jones, *J. Am. Chem. Soc.* 47, 3051 (1925); from benzyl bromide + acetamide: Erikson, *Ber.* 59, 2665 (1926); from N-benzylphthalimide + hydrazine hydrate: Ing, Manske, *J. Chem. Soc.* 129, 2348 (1926). Identity with moringine: Chakravarti, *Bull. Calcutta School Trop. Med.* 3, 162 (1955); C.A. 50, 16891c (1956).



Liquid; strongly alkaline reaction. bp 185°; bp₁₂ 90°. d_4^{25} 0.983. n_D^{20} 1.5401. Miscible with water, alcohol, ether.

Hydrochloride, $C_7H_9N.HCl$, crystals, mp 253°.

Hydroiodide, $C_7H_9N.HI$, leaflets, mp 162°.

Caution: Highly irritating to skin, mucous membranes.

USE: In organic synthesis.

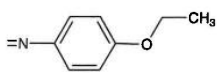
1161. Benzylaniline. N-Phenylbenzenemethanamine; N-phenylbenzylamine; benzylphenylamine. $C_{13}H_{11}N$; mol wt 183.25. C 85.21%, H 7.15%, N 7.64%. $C_6H_5CH_2NHC_6H_5$. Prep'n from benzyl alc and aniline in the presence of KOH: Sprinzak, *J. Am. Chem. Soc.* 78, 3207 (1956); from benzaldehyde and aniline in the presence of $NaBH_4$: Schellenberg, *J. Org. Chem.* 28, 3259 (1963).

Prisms, mp 37-38°. bp 306-307°. Practically insol in water; sol in alcohol, chloroform, ether.

1162. Benzyl Benzoate. Benzoic acid phenylmethyl ester; benzoic acid benzyl ester; benzylbenzenecarboxylate; Ascabine; Venzonate; Ascabiol. $C_{15}H_{12}O_2$; mol wt 212.25. C 79.23%, H 5.70%, O 15.08%. $C_6H_5COOCH_2C_6H_5$. Contained in Peru and Tolu balsams. Prep'd by the action of sodium benzoate on benzaldehyde: Kamm, Kamm, *Org. Syn. coll. vol. I*, 104 (2nd ed., 1941); by the dry esterification of sodium benzoate and benzyl chloride in the presence of triethylamine: Thorp, Nottorf, *Ind. Eng. Chem.* 39, 1300 (1947). Toxicity studies: Graham, Kuizenga, *J. Pharmacol. Exp. Ther.* 84, 358 (1945); Draize et al., *J. Pharmacol. Exp. Ther.* 93, 26 (1948). Comprehensive description: M. M. A.

Consult the Name Index before using this section.

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$N_2O \cdot HCl$, *Serenium*. Reddish. Excreted in water-soluble form. Ref: Lott and Christiansen, *J.* (1934).

il. Ethylene glycol monoethyl $C_4H_{10}O_3$; mol wt 90.12. C 1%. $HOCH_2CH_2OC_2H_5$. Manuf thanol: Faith, Keyes & Clark's Lowenheim, M. K. Moran, Eds. (ork, 4th ed., 1975) pp 403-407. h et al., *J. Ind. Hyg. Toxicol.* 23,

orless liq. d_4^{20} 0.931. bp 135°. d cup: 112°F (44°C); open cup: Misc with water, alc, ether, acees many oils, resins, waxes, etc. (Smyth).

ellulose, lacquers and dopes; in solns, dye baths; finishing leath-dye solns; increasing stability of

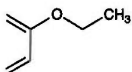
acetate. 2-Ethoxyethanol acetate; glycol monoethyl ether acetate. C 54.53%, H 9.15%, O 36.32%. Toxicity data: Smyth et al., *J.* (1941).

lor. d_4^{20} 0.975. bp 156°. Flash 2). Sol in about 6 parts water. kg (Smyth).

atoms of overexposure are irrita-ting; kidney damage; paralysis. to *Chemical Hazards* (DHHS/14).

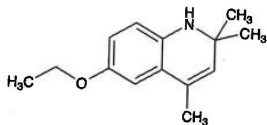
s to retard evaporation and im-

alene. Ethyl β -naphthyl ether; a "new"; β -naphthyl ethyl ether; t 172.23. C 83.69%, H 7.02%, O 3-naphthol with potassium ethyl H_2SO_4 ; Yokoyama et al., *Yaku-C.A.* 52, 10986c (1958); from β -naphthyl chloride + ethyl alcohol: *natsh.* 82, 588 (1951); from β -acetate: Patai, Bentov, *J. Am.* 2); from β -naphthol + triethyl-nic acid: Bell, U.S. pat. 2,683,-ak).



-38°. bp 28.2°. n_D^{20} 1.5932. d_4^{20} 1 water. Sol in alcohol, chloro-ene, toluene, petr ether.

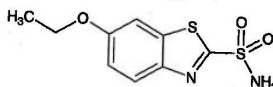
Ethoxy-1,2-dihydro-2,2,4-trimeth-ethoxy-2,2,4-trimethylquinoline; $C_{14}H_{19}NO$; mol wt 217.31. C 73.36%. Prepn: Knoevenagel, et al., *Brit. pat.* 505,113 (1939 to Iron 19, 1685 (1963). Structure: 1327. Metabolism: R. H. Wil-7, 206 (1959); J. U. Skaare, *E.* 9 (1979). Toxicity data: V. I. 601c (1979).



Yellow liquid. bp 123-125°. n_D^{25} 1.569-1.672. d_4^{25} 1.029-1.031. LD₅₀ orally in rats, mice: 1920, 1730 mg/kg (Piul'-skaya).

USE: Antioxidant in feed and food; antidegradation agent for rubber.

3801. Ethoxzolamide. 6-Ethoxy-2-benzothiazolesulfonamide; ethoxzolamide; Cardrase; Ethamide; Glaucotensil; Redupresin. $C_9H_{10}N_2O_3S_2$; mol wt 258.32. C 41.85%, H 3.90%, N 10.84%, O 18.58%, S 24.83%. Carbonic anhydrase inhibitor. Prepn: *Brit. pat.* 795,174; J. Korman, U.S. pat. 2,868,800 (1958, 1959 both to Upjohn).

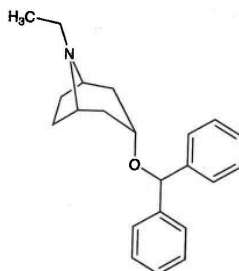


Crystals from ethyl acetate + Skellysolve B, mp 188-190.5°.

THERAP CAT: Diuretic.

THERAP CAT (VET): Diuretic.

3802. Ethylbenzotropine. endo-3-(Diphenylmethoxy)-8-ethyl-8-azabicyclo[3.2.1]octane; 3a-(diphenylmethoxy)-8-ethyl-1aH,5aH-nortropine; N-ethylnortropine benzhydryl ether; trophedrylin; N-ethyl-8-aza-3-bicyclo[3.2.1]octyl benzhydryl ether; N-ethylbenzotropine; ethylbenzotropine. $C_{22}H_{27}NO$; mol wt 321.46. C 82.20%, H 8.47%, N 4.36%, O 4.98%. Prepn: *Brit. pat.* 804,837 (1958 to Sandoz); Boehringer et al., *Brit. pat.* 824,875 (1959 to Boehringer, Ing.). Used as hydrochloride or hydrobromide salts.



Hydrochloride, $C_{22}H_{27}NO \cdot HCl$, *Ponalid*. Crystals from acetone, mp 190-191°.

Hydrobromide, $C_{22}H_{27}NO \cdot HBr$, *Ponalid*. Crystals from methanol + ether, mp 226-228°.

THERAP CAT: Anticholinergic.

3803. Ethyl Acetate. Acetic acid ethyl ester; acetic ether; vinegar naphtha. $C_4H_8O_2$; mol wt 88.11. C 54.53%, H 9.15%, O 36.32%. $CH_3COOC_2H_5$. Obtained by the slow distillation of a mixture of acetic acid, ethyl alc, and sulfuric acid: Alheritiere, Mercier, U.S. pat. 2,787,636 (1957 to Usines de Melle); Faith, Keyes, & Clark's *Industrial Chemicals*, F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 350-354. Toxicity: H. F. Smyth et al., *Am. Ind. Hyg. Assoc. J.* 23, 95 (1962).

Clear, volatile, flammable liq; characteristic fruity odor; pleasant taste when diluted. Slowly dec by moisture, then acquires an acid reaction. Absorbs water (up to 3.3% w/w). d_4^{20} 0.902; d_4^{25} 0.898. bp 77°. mp -83°. Flash pt +7.2° (open cup). Ignition temp 800°F. Explosive limits (% vol in air): 2.2 to 11.5. n_D^{20} 1.3719. Vapor density 3.04 (air = 1). One ml dissolves in 10 ml water at 25°; more sol at lower and less sol at higher temps. Misc with alc, acetone, chloroform, ether. Azeotropic mixture with water (6.1% w/w) bp

70.4°. Azeotropic mixture with water (7.8% w/w) and alc (9.0% w/w) bp 70.3°. Keep tightly closed in a cool place and away from fire. LD₅₀ orally in rats: 11.3 ml/kg (Smyth).

Caution: Potential symptoms of overexposure are irritation of eyes, nose and throat; narcosis; dermatitis. See *NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 90-117, 1990) p 104.

USE: Pharmaceutical aid (flavor); artificial fruit essences; solvent for nitrocellulose, varnishes, lacquers, and aeroplane dopes; manuf smokeless powder, artificial leather, photographic films and plates, artificial silk, perfumes; cleaning textiles, etc.

3804. Ethyl Acetoacetate. 3-Oxobutanoic acid ethyl ester; acetoacetic acid ethyl ester; acetoacetic ester; ethyl 3-oxobutanoate. $C_6H_{10}O_4$; mol wt 130.14. C 55.37%, H 7.74%, O 36.88%. $CH_3COCH_2COOC_2H_5$. Only the equilibrium mixture of the keto and enol forms is described here. Prepd from ethyl acetate by the action of sodium, sodium ethoxide, sodamide, or calcium: Inglis, Roberts, *Org. Syn. coll. vol. I*, 235 (2nd ed., 1941); Hansley, Schott, U.S. pat. 2,843,623 (1958 to Natl. Distillers); Scheibler, *Ann.* 565, 176 (1949); Gattermann-Wieland, *Praxis des Organischen Chemikers* (de Gruyter, Berlin, 4th ed., 1961) p 218. Discussion of keto-enol tautomerism: Ward, *J. Chem. Ed.* 39, 95 (1962). Toxicity study: H. F. Smyth et al., *J. Ind. Hyg. Toxicol.* 31, 60 (1949).

Liq. Agreeable odor. d_4^{20} 1.0357; d_4^{25} 1.0288; d_4^{25} 1.0213; d_4^{25} 0.9924; d_4^{25} 0.9703. mp -45°. bp₇₆₀ 180.8°; bp₄₀₀ 158.2°; bp₂₀₀ 138.0°; bp₁₀₀ 106°; bp₂₅ 81.1°; bp₅ 54.0°; bp₁₀ 28.5°. n_D^{20} 1.41937. Absorption spectrum: Morton, Rosney, *J. Chem. Soc.* 1926, 711. Flash pt, closed cup: 184°F. Sol in about 35 parts water; misc with the usual organic solvents. LD₅₀ orally in rats: 3.98 g/kg (Smyth).

Caution: Moderately irritating to skin, mucous membranes.

3805. Ethyl Acrylate. 2-Propenoic acid ethyl ester; acrylic acid ethyl ester. $C_5H_8O_2$; mol wt 100.12. C 59.98%, H 8.05%, O 31.96%. $CH_2=CHCOOC_2H_5$. Prepd from ethylene chlorohydrin or acrylonitrile, ethanol, and sulfuric acid; also by an oxo reaction from acetylene, carbon monoxide, and ethanol in the presence of suitable catalysts. See the refs under Methyl Acrylate.

Monomer, liquid, acid, penetrating odor, retained by clothing. *Lacrimator*. d_4^{20} 0.9405. fp below -72°. bp₇₆₀ 99.4°; bp₂₀ 20° (polymerizes on distn). n_D^{20} 1.404. Specific heat at -60°: 0.442 cal/g°C. Heat of vaporization 8.27 kcal/mol; heat of combustion 655.49 kcal/mol. Flash pt, open cup: 60°F (15°C). Vapor density 3.45 (air = 1). Sol in water at 20°: 2 g/100 ml. Sol of water in ethyl acrylate at 20°: 1.5 g/100 g. Sol in alcohol, ether. Azeotropes: 45.0% water = bp 81°; 56.8% ethanol = bp 76°. Easily polymerizes on standing; polymerization process speeded up by heat, light, and peroxides. If pure, the monomer can be stored below +10° without incurring polymerization.

Polymer, transparent, elastic substance. Practically no odor. Little adhesive power. Resists the usual solvents.

Caution: Potential symptoms of overexposure to the monomer are irritation of eyes, respiratory system and skin. See *NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 90-117, 1990) p 106. See also *Patty's Industrial Hygiene and Toxicology* vol. 2A, G. D. Clayton, F. E. Clayton, Eds. (Wiley-Interscience, New York, 3rd ed., 1981) p 2292-2296. This substance may reasonably be anticipated to be a carcinogen: *Seventh Annual Report on Carcinogens* (PB95-109781, 1994) p 203.

USE: The monomer in the manuf of water emulsion paint vehicles; in production of emulsion-based polymers used in textile and paper coatings, leather finish resins and adhesives. Imparts flexibility to hard films.

3806. Ethyl Alcohol. *Ethanol*; absolute alcohol; anhydrous alcohol; dehydrated alcohol; ethyl hydrate; ethyl hydroxide. C_2H_5O ; mol wt 46.07. C 52.14%, H 13.13%, O 34.73%. C_2H_5OH . Manuf: by fermentation of starch, sugar, and other carbohydrates; from ethylene, acetylene, sulfite waste liquors, and synthesis gas (CO + H₂); by hydrolysis of ethyl sulfate, and oxidation of methane. Toxicity: G. S. Wiberg et al., *Toxicol. Appl. Pharmacol.* 16, 718 (1970). Embryotoxicity in mammals: N. A. Brown et al.,

Consult the Name Index before using this section.

Science 206, 573 (1979). Possible mechanism for actions of ethanol on the brain: G. Aston-Jones *et al.*, *Nature* 296, 857 (1982). Ethanol-induced chromosomal abnormalities in mice: M. H. Kaufman, *ibid.* 302, 258 (1983). Disruption of reproductive function in female primates following alcohol self-administration: N. K. Mello *et al.*, *Science* 221, 677 (1983). Review of metabolism and toxicity: C. S. Lieber in *Reviews in Biochemical Toxicology* vol. 5, E. Hodgson *et al.*, Eds. (Elsevier, New York, 1983) pp 267-312; of pharmacology: L. Pohorecky, J. Brick, *Pharmacol. Ther.* 36, 335-427 (1988); of hepatotoxicity: C. S. Lieber, L. M. DeCarli, *J. Hepatol.* 12, 394-401 (1991). General reviews: P. Baud, "Ethyl Alcohol Industry" in Grignard, *Traité de Chimie Organique* vol. 5 (Masson, 1937) pp 841-975; Zabel, *Chem. Ind.* (now *Chem. Week*) 64, 212 (1949); Faith, Keyes & Clark's *Industrial Chemicals*, F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 355-364; P. D. Sherman, P. R. Kavasmaneck, "Ethanol" in Kirk-Othmer *Encyclopedia of Chemical Technology* vol. 9 (Interscience, New York, 3rd ed., 1980) pp 338-380.

Clear, colorless, very mobile, flammable liquid; pleasant odor; burning taste. Absorbs water rapidly from air. d_{40}^{20} 0.789. bp 78.5°. mp -114.1°. n_D^{20} 1.361. Flash pt, closed cup: 13°C. Miscible with water and with many organic liquids. Keep tightly closed, cool, and away from flames. LD₅₀ in young, old rats (g/kg): 10.6, 7.06 orally (Wiberg).

The terms 95% alcohol and alcohol (when used alone) refer to a binary azeotrope having a distillate composition of 95.57% ethyl alcohol (by wt) and bp 78.15°. Alcohol, USP is specified as containing not less than 92.3% and not more than 93.8% by weight, corresponding to not less than 94.9% and not more than 96.0% by vol of C₂H₅OH at 15.56°. d_{40}^{20} 0.810; d 0.816 at 15.56° (60°F). Diluted alcohol, prep'd from equal vols 95% alcohol and water, contains about 41.5% by wt or about 48.9% by vol of C₂H₅OH. d_{40}^{20} 0.931; d 0.936 at 15.56° (60°F). See U.S.P. XXI, 22, 1530 (1985).

Caution: Nausea, vomiting, flushing, mental excitement or depression, drowsiness, impaired perception, incoordination, stupor, coma, death may occur. *cf.* *Clinical Toxicology of Commercial Products*, R. E. Gosselin *et al.*, Eds. (Williams & Wilkins, Baltimore, 5th ed., 1984) Section III, pp 166-171.

USE: Most ethyl alcohol is used in alcoholic beverages in suitable dilutions. Other uses are as solvent in laboratory and industry, in the manufacture of denatured alcohol, pharmaceuticals (rubbing compds, lotions, tonics, colognes), in perfumery, in organic synthesis. Octane booster in gasoline. Pharmaceutical aid (solvent).

THERAP CAT: Antiseptic.

THERAP CAT (VET): Antiseptic. To destroy nerve tissue. Solvent and dehydrating agent.

3807. Ethyl Alcohol, Denatured. Denatured alcohol. Ethyl alcohol to which has been added some substance or substances which, while allowing the use of the alcohol in the most varied industries and arts, renders it entirely unfit for consumption as a beverage. The most commonly used denaturants, either alone or in combination, are the following: Methanol, camphor, Aldehol, amyl alcohol, gasoline, isopropanol, terpineol, benzene, castor oil, acetone, nicotine, aniline dyes, ether, cadmium iodide, pyridine bases, sulfuric acid, kerosene, diethyl phthalate. *Formula 1* is 5 gallons approved wood alcohol added to 100 gal of 95% ethanol. *Formula 2B* is 0.5 gal benzene added to 100 gal of 95% ethanol. Similarly *formula 3A* contains 5 gal commercial methanol, *formula 6B* contains 0.5 gal pyridine bases, *formula 12A* 5 gal benzene, *formula 13A* 10 gal ethyl ether, *formula 19A* 4 gal methyl isobutyl ketone and 1 gal kerosene, *formula 20* 5 gal crude chloroform, *formula 23A* 10 gal acetone, *formula 28* 10 gal benzene, *formula 28A* 1 gal gasoline, *formula 30* 10 gal methanol, *formula 32* 5 gal ethyl ether, *formula 33* 30 lbs methyl violet, *formula 35A* 5 gal ethyl acetate, *formula 39C* 1 gal diethyl phthalate; *formula 44* contains 20 gal *n*-butanol. Additional permissible formulas are given in *Appendix to Regulations No. 3, Formulae for Completely and Specially Denatured Alcohol*, published by the U.S. Treasury Dept., Bureau of Industrial Alcohol. Reprinted in N. A. Lange, *Handbook of Chemistry*.

Caution: Denaturants, particularly methanol, may modify and increase toxic symptoms caused by ingestion and exposure to fumes.

3808. Ethylamine. *Ethanamine*; monoethylamine; aminoethane. C₂H₇N; mol wt 45.08. C 53.28%, H 15.65%, N 31.07%. C₂H₅NH₂. Prep'n from ethyl iodide + liq ammonia: Watt, Otto, *J. Am. Chem. Soc.* 69, 836 (1947); from ethanol + ammonia: Davies *et al.*, U.S. pat. 2,609,394 (1952 to ICI); Lemon, Myerly, U.S. pat. 3,022,349 (1962 to Union Carbide). Toxicity study: H. F. Smyth *et al.*, *Arch. Ind. Hyg. Occup. Med.* 10, 61 (1954).

Flammable, liq; ammonia odor; strong alkaline reaction. d_{40}^{20} 0.689. bp 16.6°. Solidif -80°. Miscible with water, alcohol, ether. Keep tightly closed and in cold place. LD₅₀ orally in rats: 0.40 g/kg (Smyth).

Hydrochloride, C₂H₇N.HCl, crystals from ethanol + water, mp 110°. d 1.22. Soluble in 0.4 part water; freely sol in alcohol; slightly sol in chloroform or acetone. Practically insol in ether. Keep well closed.

Hydride, C₂H₅NH, hygroscopic crystals, mp 188°. d 2.10. Freely sol in water or alcohol. Practically insol in chloroform, ether. Keep well closed and protected from light.

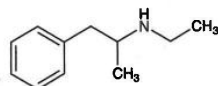
Oleate, C₂H₇N.C₁₈H₃₅O₂, *ethanamine (Z)-9-octadecenoate, Etalate*. Commercial prep'n is a 5% soln with 2% benzyl alcohol as anodyne.

Caution: Potential symptoms of overexposure are irritation of eyes; skin burns; respiratory irritation; dermatitis. See NIOSH Pocket Guide to Chemical Hazards (DHHS/NIOSH 90-117, 1990) p 106.

USE: In resin chemistry; stabilizer for rubber latex; intermediate for dyestuffs, medicinals; in oil refining; in organic syntheses.

THERAP CAT: Oleate as a sclerosing agent.

3809. N-Ethylamphetamine. *N-Ethyl-α-methylbenzene-ethanamine*; *N-ethyl-α-methylphenethylamine*; *N-ethyl-ω-phenylisopropylamine*; 2-ethylamino-1-phenylpropane; Adiparhol; Apetinin. C₁₁H₁₇N; mol wt 163.26. C 80.93%, H 10.50%, N 8.58%. Prep'n: Keil, Dobke, Ger. pat. 767,263 (1952 to Theodor H. Temmler); Leonard *et al.*, *J. Am. Chem. Soc.* 80, 4858 (1958). Separation of isomers: Brit. pat. 814,339 (1959 to Sterling Drug).



bp₁₄ 104.5-106°. n_D^{25} 1.4986.

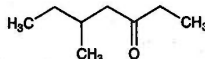
d-Form hydrochloride, C₁₁H₁₇N.HCl, mp 154-156°. [α]_D²⁵ +17.2° (c = 2 in water).

l-Form hydrochloride, C₁₁H₁₇N.HCl, mp 155-156°. [α]_D²⁵ -17.3° (c = 2 in water).

Note: This is a controlled substance (stimulant) listed in the U.S. Code of Federal Regulations, Title 21 Part 1308.11 (1995).

THERAP CAT: Anorexic.

3810. Ethyl Amyl Ketone. *5-Methyl-3-heptanone*; amyl ethyl ketone; EAK. C₈H₁₆O; mol wt 128.21. C 74.94%, H 12.58%, O 12.48%. Review: Buller, *Ind. & Eng. Chem.* 48, 1323 (1956).



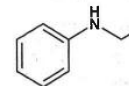
Liquid. Mild fruity odor. d_{40}^{20} 0.820-0.824. One gallon weighs 6.83 lbs at 20°. bp₇₆₀ 157-162°. Flash pt 59° (138°F). Evaporation rate 0.3 (*n*-butyl acetate = 1.0). n_D^{20} 1.4195. Slightly miscible with water. Compatible with alcohols, ketones, ethers, many other organic solvents.

Caution: Narcotic in high concns.

USE: Solvent for nitrocellulose-alkyd, nitrocellulose-maleic, and vinyl resins.

3811. Ethylaniline. *N-Ethylbenzenamine*; ethylphenylamine. C₉H₁₁N; mol wt 121.18. C 79.29%, H 9.15%, N

11.56%. Produced by heating ar alcohol at 180°.



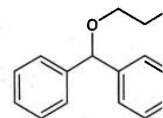
Very refractive liquid; rapidly b sure to light and air. Aniline-like o below 80°. bp 204.5°. mp -63°. water; miscible with alc, ether and vents. Keep well closed and protecte in rats: 1.1 g/kg.

3812. Ethylbenzene. C₈H₁₀; n H 9.49%. C₆H₅C₂H₅. Prep'n from menses, Ber. 46, 1838 (1913); Gat des organischen Chemikers (de G 1961) p 332. By Huang-Minlor Kishner reduction: A. I. Vogel, *P* (Longmans, 3rd ed., 1959) p 516. C. Gibbons *et al.*, *J. Am. Chem Manuf*: Faith, Keyes & Clark's *Lowenheim*, M. K. Moran, Eds. York, 4th ed., 1975) pp 365-370.

Colorless liquid; flammable. d_{40}^{20} -95.01°. n_D^{20} 1.4932. Flash pt, Practically insol in water. Misc vents. LD₅₀ orally in rats: 5.46 g

Caution: Potential symptoms o tion of eyes and mucous membrai narcosis, coma. See NIOSH P Hazards (DHHS/NIOSH 90-117, **USE:** For conversion to styrene n

3813. Ethylbenzhydramine. *diethylethanamine*; 2-(benzhydry ethylaminoethyl benzhydryl ether diethylethylamine; benzhydryl 2- etanautine. C₁₅H₂₅NO; mol wt 28. N 4.94%, O 5.65%. Prep'n: Mart 799 (1946 to Geigy); Rieveschl, U. Parke, Davis).



bp_{0.15} 140-142°.

Hydrochloride, C₁₅H₂₅NO.HCl, alcohol + ethyl acetate, mp 140°. water; sol in alcohol, acetone, chl in benzene, ether. pH of 1% aq s Methyl iodide, C₁₅H₂₅NO.CH₃I **THERAP CAT:** Anticholinergic; a

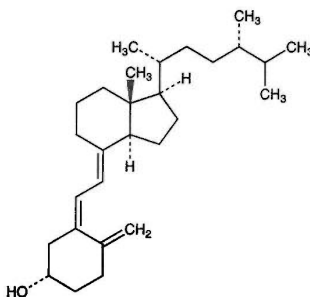
3814. Ethyl Benzoate. Benz O₂; mol wt 150.18. C 71.98%, H COOC₂H₅.

Colorless, clear, refractive lic cause cough. d_{40}^{20} 1.050. bp 211-2 Almost insol in water; miscible ether, petr ether. LD₅₀ orally in *al.*, *Arch. Ind. Hyg. Occup. Med.*

USE: In perfumery under the i manuf of *Peau d'Espagne*; artificie

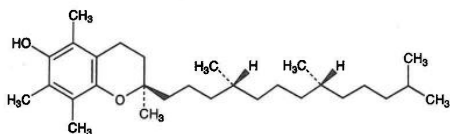
3815. Ethyl Benzoylacetate acid ethyl ester. C₁₁H₁₂O₃; mol 6.29%, O 24.97%. C₆H₅COCH₂C Liquid; pleasant odor; becomes and light. d_{15}^{20} 1.122. bp 265-270

11.63%, O 4.01%. Prep'd from 22:23-dihydroergosterol by irradiation with light of the magnesium arc: Windaus, Trautmann, *Z. Physiol. Chem.* 247, 185 (1937). Synthesis: P. J. Kocienski et al., *J. Chem. Soc., Perkin Trans. I* 1979, 1290.



Platelets from dil acetone, mp 96-98°. Originally given as mp 107-108°, see Windaus, Guntzel, *Ann.* 538, 122 (1939). $[\alpha]_D^{25} +89.3^\circ$ (c = 0.47 in acetone). uv max: 265 nm. Not precipitated by digitonin. Practically insol in water. Sol in the usual organic solvents except petr ether; slightly sol in vegetable oils.

10159. Vitamin E. [2R*(4R*,8R*)]-3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol; 2,5,7,8-tetramethyl-2-(4',8',12'-trimethyltridecyl)-6-chromanol; α -tocopherol; (+)- α -tocopherol; 5,7,8-trimethyltolcol; antisterility vitamin. $C_{55}H_{100}O_2$; mol wt 430.71. C 80.87%, H 11.70%, O 7.43%. Found largely in plant materials. Present in highest concns (0.1-0.3%) in wheat germ, corn, sunflower seed, rapeseed, soybean oils, alfalfa and lettuce. Natural α -tocopherol is usually found with β - and γ -tocopherols, q.v. Isoln from wheat germ: Evans et al., *J. Biol. Chem.* 113, 319 (1936). Structure: Fernholz, *J. Am. Chem. Soc.* 59, 1154 (1937); 60, 700 (1938). Synthesis: Karrer et al., *Helv. Chim. Acta* 21, 520, 820 (1938); Bergel et al., *J. Chem. Soc.* 1938, 1382; Smith et al., *Science* 88, 37 (1938); Smith, Sprung, *J. Am. Chem. Soc.* 65, 1276 (1943). Recent syntheses: N. Cohen et al., *Helv. Chim. Acta* 61, 837 (1978); *idem*, *J. Am. Chem. Soc.* 101, 6710 (1979); R. Barnier, M. Schmid, *Helv. Chim. Acta* 62, 2384 (1979). Abs confg of natural α -tocopherol: Mayer et al., *ibid.* 46, 963 (1963). Stereoselective synthesis of the side chain: C. H. Heathcock, E. T. Jarvi, *Tetrahedron Letters* 23, 2825 (1982). Review of industrial processes: Rubel, *Vitamin E Manufacture* (Noyes Dev. Corp., Park Ridge, N.J., 1969). Reviews: *The Vitamins* Vol. 5, W. H. Sebrell, R. S. Harris, Eds. (Academic Press, New York, 1972) pp 165-317; J. M. Bieri, P. M. Farrell, *Vitam. Horm. (New York)* 34, 31-75 (1976). Book: *Ann. N.Y. Acad. Sci.* 393, entitled "Vitamin E: Biochemical, Hematological and Clinical Aspects", B. Lubin, L. J. Machlin, Eds. (1982) 506 pp. Review of medical uses: J. G. Bieri et al., *N. Engl. J. Med.* 308, 1063-1071 (1983).



$[\alpha]_D^{25} -3.0^\circ$ (benzene); $[\alpha]_D^{25} +0.32^\circ$ (alc).

Succinate, *Vitamin E acid succinate*. Prep'n: Demole et al., *Helv. Chim. Acta* 22, 65 (1939); McArthur, Watson, *Can. Chem. Process Inds.* 23, 350 (1939); Baxter et al., *J. Am. Chem. Soc.* 65, 918 (1943). Needles from petr ether, mp 76-77°. uv max (ethanol): 286 nm ($E_{1\%}^{1cm}$ 38.5). Practically insol in water.

Nicotinate, $C_{55}H_{103}NO_3$, *Hijuven*, *Juvela Nicotinate*, *Renascin*.

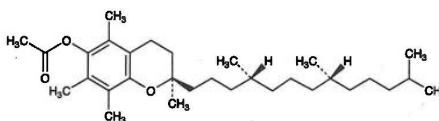
dl-Form, slightly viscous, pale yellow oil. Natural α -tocopherol has been crystallized, mp 2.5°-3.5°. d_4^{25} 0.950;

bp_{0.1} 200-220°; n_D^{25} 1.5045. uv max: 294 nm ($E_{1\%}^{1cm}$ 71). Practically insol in water. Freely sol in oils, fats, acetone, alcohol, chloroform, ether, other fat solvents. Stable to heat and alkalis in the absence of oxygen. Not affected by acids up to 100°. Slowly oxidized by atm oxygen, rapidly by ferric and silver salts. Gradually darkens on exposure to light.

USE: As an antioxidant in vegetable oils and shortening. THERAP CAT: Treatment of vitamin E deficiency.

THERAP CAT (VET): Nutritional factor. Interrelationship with selenium. (Prevents muscle degeneration, also encephalomalacia and exudative diathesis.) Has been used to promote fertility.

10160. Vitamin E Acetate. [2R*(4R*,8R*)]-3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol acetate; 2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-6-chromanol acetate; α -tocopherol acetate; α -tocopheryl acetate; $C_{57}H_{102}O_3$; mol wt 472.75. C 78.76%, H 11.09%, O 10.15%. Prep'n from *dl*- α -tocopherol and acetic anhydride: Surmatis, Weber, U.S. pat. 2,723,278 (1955 to Hoffmann-La Roche). Prep'n of *d*- and *l*-forms: Robeson, Nelan, *J. Am. Chem. Soc.* 84, 3196 (1962). Stereoselective synthesis: K.-K. Chan et al., *J. Org. Chem.* 43, 3435 (1978). Total synthesis of all eight stereoisomers: N. Cohen et al., *Helv. Chim. Acta* 64, 1158 (1981). Comprehensive description: B. C. Rudy, B. Z. Senkowski, *Anal. Profiles Drug Subs.* 3, 111-126 (1974).



dl-Form, *Detulin*, *Ephynal*, *Eprolin*, *Epsilan-M*, *Eusovit*, *E-Vimin*, *Evion*, *Juvela*, *OptoVit-E*, *Toco 500*, *Vitagutt*. Pale yellow, viscous liquid. mp -27.5°. d_4^{25} 0.9533. bp_{0.01} 184°; bp_{0.025} 194°; bp_{0.3} 224°. n_D^{20} 1.4950-1.4972. uv max (cyclohexane): 285.5 nm. Practically insol in water. Freely sol in acetone, chloroform, ether. Less readily sol in alc. Unlike the free vitamins, the acetate is practically unaffected by the oxidizing influence of air, light, and ultraviolet light.

d-Form, [2R-[2R*(4R*,8R*)]-3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol acetate, *E-Victrat*, *Spondylvit*, *Tocopherex*. Crystals, mp 28°. $[\alpha]_D^{25} +0.25^\circ$ (c = 10 in chloroform); $[\alpha]_D^{25} +3.2^\circ$ (in ethanol). *l*-Form, crystals, mp 23°. $[\alpha]_D^{25} -2.0^\circ$ (in ethanol).

Note: The international unit of vitamin E is equal to one mg of standard *dl*- α -tocopheryl acetate. The *d*-form is more active: 1 mg = 1.36 I.U. *l*- α -Tocopheryl acetate has 42% of the activity of *d*- α -tocopheryl acetate in the rat hemolysis test. Based on this activity a potency ratio of 1.4:1.0 for *d*- α -tocopheryl acetate compared to *dl*- α -tocopheryl acetate has been established.

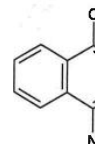
THERAP CAT: Vitamin.

THERAP CAT (VET): Vitamin.

10161. Vitamin K. General term referring to a group of naphthoquinone derivatives required for the bioactivation of proteins involved in hemostasis. The designation "K" was derived from the German "Koagulationsvitamin." Vitamin K compds are classified into 3 groups: *phyloquinone* (K_1), q.v., found in green plants; *menaquinones* (K_2), q.v., primarily produced by intestinal bacteria; and *menadione* (K_3), q.v., and derivatives which are synthetic, lipid soluble compounds. Reduced *in vivo* to *dihydrovitamin K* (KH_2) which serves as a coenzyme in the conversion of glutamic acid residues to γ -carboxyglutamic acid (Gla), q.v., in the post-translational modification of blood coagulation factors II, VII, IX and X, q.v., and the anticoagulant proteins C and S. Other Gla-containing proteins, such as the bone matrix protein, osteocalcin, q.v., have been identified in a wide variety of tissues. This γ -carboxylation is accompanied by the oxidation of KH_2 to *vitamin K epoxide* which is then recycled back to vitamin K. Discovery: H. Dam, *Biochem. Z.* 215, 475 (1929); 220, 158 (1930); *Nature* 135, 652 (1935). Historical survey: H. Dam, *Vit. Horm.* 24, 295-306 (1966). Menadione and phyloquinone are metabolized by animals

to menaquinone-4: C. Marti, *Brit. J. Nutr.* 72, 415 (1994). Friedrich in *Vitamins* (de Gr 285-338. Review of metabolism: M. J. Shearer, *Blood* 1 Suttie, *J. Am. Diet. Assoc.* 92, 5 of action: P. Dowd et al., (1994); of pharmacology and *et al.*, *Drugs* 49, 376-387 (1994). J. Shearer, *Lancet* 345, 229-23.

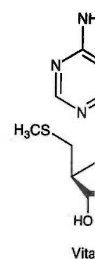
10162. Vitamin K₃. 4-Amino-2-methyl-1-naphthol; naphthalene; 2-methyl-4-aminomethyl-4-amino-1-naphthol; thylamine; Synkamin. $C_{11}H_9NO$ 76.28%, H 6.40%, N 8.09%. α -naphthalene or from menadione 458 (1940); 60, 373 (1941); V (1942); 62, 75 (1943). Use: Steele, *Food Technol.* 12, 501 (



Hydrochloride, $C_{11}H_{11}NO \cdot HCl$, darkens at 262°, dec 2 violet on exposure to air and Slightly sol in alc. Insol in eth N-Acetyl analog, $C_{13}H_{13}NO$ naphthol, K-Vitrat. Needles, n USE: Food preservative.

THERAP CAT: Vitamin (prothi

10163. Vitamin(s) L. Facts lactation. Vitamin L₁: See o-A L₂ was shown to be 7-[tetrahydropyrimidin-2-yl]aden Papers Inst. Phys. Chem. Reser C.A. 41, 6317c (1947). Manu 7244(62) and 16,015 (69), C. 77, 102146j (1972).



10164. Vitamin T. Tegotin vitamin T Goetsch; Goetsch's v of growth-promoting substance termites: Goetsch, *Oesterr. Zo obtainable from roaches, yeast cedure has never been describer plexes" from yeast: Koch et a to Aschaffenburg Zellstoffwe Vitamin T may be a mixtur growth-promoting factors: Ko (1951). Polemic by Barkow, G*

10165. Vitamin U. (S)-(- dimethyl sulfonium chloride; chloride; MMSC; Cabagin-U; $C_{10}H_{12}S_2$; mol wt 199.70. C 36;