

The Merck Index OnlineSM

FILE DESCRIPTION

The Merck Index OnlineSM is the online version of the monographs in the printed 14th Edition of *The Merck Index* (a U.S. publication, Whitehouse Station, N.J., USA), an internationally recognized, one-volume encyclopedia of chemicals, drugs, and biologicals. Each monograph in the encyclopedia (each record in the database) discusses a single chemical entity or a small group of very closely-related compounds. Updates contain material not yet available in print.

Records contain:

- chemical, common, generic and systematic names (including CAS[®] names)
- trademarks and associated companies
- CAS[®] Registry Numbers
- molecular formulae, weights and percentage composition
- capsule statements identifying compound classes and scientific significance
- chemical, biomedical and patent literature references
- physical and toxicity data
- therapeutic and commercial uses
- caution and hazard information

The 14th Edition also contains "retired" records from earlier editions of *The Merck Index* which still contain valuable information but are no longer being updated with new information

SUBJECT COVERAGE

- human and veterinary drugs
- biotech drugs and monoclonal antibodies
- substances used for medical imaging
- biologicals and natural products
- plants and herbal medicines
- agricultural chemicals (including pesticides and herbicides)
- organic and inorganic chemicals used in commerce and research
- laboratory reagents and catalysts
- dyes, colors and indicators
- environmentally significant substances

SOURCES

Records contain active citations to and information from approximately 800 international chemical, biomedical, and clinical journals; patents issued by 30 countries; books; proceedings; and other standard reference works. Retired citations which are also included but are not longer updated.

TIPS

USE FILE 304

to find concise descriptions of specific chemicals, drugs, or biologicals.

USE NA= or /NA

to locate a substance record by its systematic name, synonym, or brand name, particularly when you don't know which kind of name you have.

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EXPAND NA=ENALAPRIL  
SELECT PHENYLPROPYL/NA
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USE MAP RN

to create a SearchSave of the CAS[®] Registry Numbers for further searching in other chemistry files.

USE /ACTIVE

to restrict a search in file 304 to 14th Edition records.
SELECT CO=AVENTIS/ACTIVE

DIALOG FILE DATA

Inclusive Dates: Late 19th Century to the present

Update Frequency: Semi-Annual

File Size: 11338 records as of July 2009

CONTACT

The Merck Index Online is produced by Merck & Co., Inc., Whitehouse Station, NJ, USA. Questions concerning file content should be directed to:

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File 304
SAMPLE RECORD

The Merck Index OnlineSM

File 304:THE MERCK INDEX ONLINE(SM) 2009/S1
(c) 2009 Merck & Co, Inc, All rts rsvd

AN=,/MN,MN= 08428 Monograph Name: Selegiline
RN= CAS REGISTRY NUMBER: 14611-51-9
MF=,/MW= MOLECULAR FORMULA: C13H17N MOLECULAR WEIGHT: 187.28
MOLECULAR COMPOSITION: C 83.37%, H 9.15%, N 7.48%
/CN,CN=,/NA,NA=,/DE C.A. CHEMICAL NAME(s): (alphaR)-N,alpha-Dimethyl-N-2-propyl-1-ylbenzeneetha
namine
SYNONYMS:
/SY,SY=,/NA,NA=,/DE L-(-)-N,alpha-dimethyl-N-2-propynylphenethylamine ; L-N-(2-phenylisopropyl
)-N-methylprop-2-ynylamine ; (-)-deprenil ; L-deprenyl
BRAND NAME (and COMPANY):
/TN,TN=,/CO,CO= Emsam (Somerset)
/SO,SO= LITERATURE REFERENCES:
Monoamine oxidase-B inhibitor related structurally to pargyline, q.v.
Prepn of racemate: FR 1368136; GB 1031425 (1964, 1966 both to Chinoin);
of (-)-form: NL 6605956; GB 1153578 (1966, 1969 both to Chinoin); J. S.
Fowler, J. Org. Chem. 42, 2637 (1977)
(<http://dx.doi.org/10.1021/jo00435a026>) (<http://www.ncbi.nlm.nih.gov/pubmed/874623>). Pharmacology and toxicology of racemate: J. Knoll et al., Arch.
Int. Pharmacodyn. 155, 154 (1965)
(<http://www.ncbi.nlm.nih.gov/pubmed/4378644>); of isomers: K. Magyar et
al., Acta Physiol. Acad. Sci. Hung. 32, 377 (1967)
(<http://www.ncbi.nlm.nih.gov/pubmed/5595908>). Review of pharmacology: E.
H. Heinonen, R. Lammintausta, Acta Neurol. Scand. Suppl. 136, 44 -59 (1991)
(<http://www.ncbi.nlm.nih.gov/pubmed/1686954>); of efficacy in
Parkinson's disease: D. W. Robin, Am. J. Med. Sci. 302, 392 -395 (1991)
(<http://dx.doi.org/10.1097/0000441-199112000-00014>) (<http://www.ncbi.nlm.nih.gov/pubmed/1772127>); K. L. Poston, C. Waters, Expert Opin.
Pharmacother. 8, 2615 -2624 (2007)
(<http://dx.doi.org/10.1517/14656566.8.15.2615>) (<http://www.ncbi.nlm.nih.gov/pubmed/17931095>). Review of veterinary use in canine cognitive
dysfunction: W. W. Ruehl, B. L. Hart in Psychopharmacology of Animal
Behavior Disorders, N. H. Dodman, L. Shuster, Eds. (Blackwell Sci.,
Malden, Mass., 1998) pp 283-304. Review of transdermal selegiline in major
depressive disorder: D. S. Robinson, J. D. Amsterdam, J. Affect. Disord.
105, 15 -23 (2008)
(<http://dx.doi.org/10.1016/j.jad.2007.04.024>) (<http://www.ncbi.nlm.nih.gov/pubmed/17568687>).
PATENT INFORMATION:
PN= FR 1368136; GB 1031425; NL 6605956; GB 1153578
PHYSICAL DATA:
/PP,PP= Oil, bp0.8 92-93. nD20 1.5180.
PHYSICAL DATA:
BT=,BP= BOILING POINT: bp0.8 92-93
RE=,RI= REFRACTIVE INDEX: nD20 1.5180
DERIVATIVE INFORMATION:
? /SY,SY=,/NA,NA=,/DE SUBSTANCE: Selegiline Hydrochloride
RN= DERIVATIVE CAS RN: 14611-52-0
MF= DERIVATIVE MOLECULAR FORMULA: C13H17N.HCl
MW= MOLECULAR WEIGHT: 223.74
MOLECULAR COMPOSITION: C 69.79%, H 8.11%, N 6.26%, Cl 15.85%
/TN,TN=,/CO,CO= DERIVATIVE BRAND NAME (COMPANY): Anipryl (Deprenyl); Antiparkin (Viatris);
Amindan (Desitin); Carbex (Endo); Deprenyl (Orion); Egibren (Chiesi);
Eldepryl (Somerset); Jumex (Chiesi); Movergan (Orion); Otrassel
(Cephalon); Plurimen (Viatris); Seledat (Master); Selegam (Hexal);
Selepark (Betapharm); Selgimed (Hennig); Xilopar (Cephalon); Zelapar
(Valeant)
/PP,PP= DERIVATIVE PHYSICAL DATA: Crystals, mp 141-142. (alpha)25/D: -10.8 (c =
6.48 in water). Freely sol in water, chloroform, methanol. LD50 in rats
(mg/kg): 81 i.v., 280 s.c. (Magyar).
MELTING POINT: 141-142
MP=,MT= OPTICAL ROTATION: (alpha)25/D: -10.8 (c = 6.48 in water)
OP=,OT= LD50: LD50 in rats (mg/kg): 81 i.v., 280 s.c. (Magyar)
LD= SUBSTANCE: Selegiline (+/-)-Form
/SY,SY=,/NA,NA=,/DE DERIVATIVE CAS RN: 2323-36-6;
RN= DERIVATIVE SYNONYMS: Deprenyl ; phenylisopropyl-N-methylpropinylamine
/SY,SY=,/NA,NA=,/DE DERIVATIVE PHYSICAL DATA: Oil, bp5 104-110. nD20 1.5229.
/PP,PP= BOILING POINT: bp5 104-110
BP=,BT= REFRACTIVE INDEX: nD20 1.5229
RE=,RI= SUBSTANCE: Selegiline (+/-)-Form hydrochloride
/SY,SY=,/NA,NA=,/DE DERIVATIVE CAS RN: 2079-54-1;
RN= DERIVATIVE DRUG CODES: E-250
/SY,SY=,/NA,NA=,/DE

SAMPLE RECORD (cont'd)

/PP,PP=	DERIVATIVE PHYSICAL DATA: Crystals from ethanol + ether, mp 131-131.5. LD50 in rats (mg/kg): 63 i.v., 126 s.c., 385 orally (Knoll).
MP=,MT=	MELTING POINT: 131-131.5
LD=	LD50: LD50 in rats (mg/kg): 63 i.v., 126 s.c., 385 orally (Knoll)
/Tc,RC=	THERAPEUTIC CATEGORY: Antiparkinsonian; antidepressant.
/TC,TV=	THERAPEUTIC CATEGORY VET: In treatment of canine cognitive dysfunction syndrome.
/KS,KW=	KEYWORDS: Antiparkinsonian; Monoamine Oxidase Inhibitor; Antidepressant; Others
/DP,RP=	REFERENCE KEYS PRESENT: Pharmacology; Prepn; Review; Toxicology; Use; Patent number
/DP,DP=	DATA KEYS PRESENT: Boiling point; Refractive Index; Patent Number; Molecular Weight; Therapeutic Category; Therapeutic Category Vet
/DP,DP=	DATA KEYS PRESENT IN DERIVATIVE: Melting point; Boiling point; Optical Rotation; Refractive Index; Lethal Dose

SEARCH OPTIONS

BASIC INDEX

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
—	—	All Basic Index Fields	Word	S ALPHA(W)DIMETHYL S METHYL
/CN	CN	CA Chemical Name ^{1,2}	Segment & Word & Phrase	S PROPYL/CN S PHENYLPROPYL(1W)ALANYL/CN S "S)-1-(N-(1-(ETHOXYCARBONYL)-3"?/CN
/CO	CO	Company Name ¹	Word	S MERCK/CO
/DE	DE	Chemical Name	Segment & Word & Phrase	S PHENYL/DE S SELEGILINE(W)HYDROCHLORIDE/DE S SELEGILINE HYDROCHLORIDE/DE
/DP	DP	Data Present ^{1,3}	Word	S MELTING(W)POINT
/EC	MF	Element Count ^{1,2}	Phrase	S (C13(S)H17)/EC
/KW	KW	Keywords ¹	Word	S ANTIPARKINSONIAN/KW
/MN	MN	Monograph Name ^{1,2}	Segment & Word & Phrase	S CHLORIDE/MN S SELEGILINE/MN S SELEGILINE HYDROCHLORIDE/MN
/NA	NA	Chemical Name ^{1,2}	Segment & Word & Phrase	S PHENYL/NA S L(W)DEPRENYL/NA S ENALAPRIL MALEATE/NA
/NT	NT	Notes, Cautions, and Uses	Word	S MORDANT(S)CATALYST/NT
/PP	PP	Physical Property Information ³	Word	S WHITE(1W)POWDER/PP
/SO	SO	Sources/References ^{4,5}	Word	S J(W)AFFECT?(W)DISORD?/SO S U(W)S(W)PAT?/SO
/SY	SY	Synonyms Including Brand Names and Drug Codes ^{1,2}	Segment & Word & Phrase	S ANITPARKIN/SY,DERIV S CO(W)RENITEC/SY S CO-RENITEC/SY
/TC	TC	Therapeutic Category ⁶	Word	S ANTIDEPRESSANT/TC
/TN	TN	Brand Name ^{1,2}	Segment & Word & Phrase	S EMSAM/TN S CARBEX/TN,DERIV S CO-RENITEC/TN

¹ Searchable in the Basic Index and in the Additional Indexes. Any numeric values are searchable in the Basic Index using the (W) operator, e.g. S 143(W)144(W)5/PP

² All chemical names are indexed as complete phrases, individual words, and chemically significant segments of words. Use /FW to restrict retrieval to the complete term, e.g., S ETHANE/FW to only select ethane as a single word rather than as a segment of a larger chemical term, such as trichloroethane.

³ Searchable as /DP in the Basic Index and using DP= or RP= in the Additional Indexes.

⁴ Includes Monograph Name (/MN, MN=), C.A. Names (/CN, CN=), Brand Names (/TN, TN=), Derivative Names (/DERIV), Drug Codes (/SY, SY=), and Synonyms (/SY, SY=).

⁵ Recent records include the URLs which can be used to locate the original article based on the DOI (digital object identifier) or the PUBMED identifier. Although not provided as hot links, the URL can be pasted into any internet browser by copying the URL string contained in the record.

⁶ Searchable using /TC in the Basic Index and using TC= or TV= in the Additional Indexes.

ADDITIONAL INDEXES

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
AN=	AN	DIALOG Accession Number	Phrase	S AN=08428
AN=	AN	THE MERCK INDEX Monograph Number	Phrase	S AN=08428 S AN=1310215/RETIRED
BP=	BP	Boiling Point (Celsius) ^{1,7}	Numeric	S BP=92.000
BT=	BP	Boiling Point Text ¹	Word	S BT=BP5
CN=	CN	C.A. Chemical Name ¹	Phrase	S CN=S)-1-(N-(1-(ETHOXYCARBONYL?
CO=	CO	Company Name ¹	Phrase	S CO=MERCK & CO?
DN=	DN	Relative Density ^{1,7}	Numeric	S DN=1.0000
DP=	DP	Data Present ^{1,3}	Phrase	S DP=(BOILING POINT AND MELTING POINT)
DT=	DN	Density Text ¹	Word	S DT=SUPERCOOLED AND DN=1.0
EC=	MF	Element Count ¹	Phrase	S EC=(C0013 AND H0017) S EC=N0001:N0005
FF=	FP	Flash Point (Fahrenheit) ^{1,7}	Numeric	S FF=84.2
FP=	FP	Flash Point (Celsius) ^{1,7}	Numeric	S FP=29
FT=	FP	Flash Point Text ¹	Word	S FT=(CLOSED(W)CUP)
KW=	KW	Keywords ¹	Word	S KW=MONOAMINE(W)OXIDASE)
LD=	LD	Lethal Dose (LD50) ¹	Word	S LD=RATS
ME=	—	Molecular Elements	Phrase	S ME=CHN
MF=	MF	Molecular Formula	Phrase	S MF=C13H17N.HCL
MN=	MN	Monograph Name ¹	Phrase	S MN=SELEGILINE
MP=	MP	Melting Point ^{1,7}	Numeric	S MP=141.000
MT=	MP	Melting Point Text ¹	Word	S MT=DEG
MW=	MW	Molecular Weight ⁷	Numeric	S MW=187.26
NA=	NA	Chemical Name ^{1,4}	Phrase	S NA=ENALAPRIL
OP=	OP	Optical Rotation ^{1,7}	Numeric	S OP=10.1:10.9
OT=	OP	Optical Rotation Text ¹	Word	S OT=(ALPHA(S)22(S)546)
PN=	PN	Patent Number ¹	Phrase	S PN=gb 1031425
PP=	PP	Physical Property Information ¹	Word	S PP=(OFF(W)WHITE AND POWDER)
RE=	RE	Refractive Index ^{1,7}	Numeric	S RE=1.518:1.519
RI=	RE	Refractive Index Text ¹	Word	S RI=(ND(W)20)
RN=	RN	CAS(R) Registry Number	Phrase	S RN=14611-51-9 S RN=14611-51-9/MAIN S RN=2323-36-6/DERIV S RP=PHARMACOLOGY
RP=	RP	References Present ³	Phrase	S RP=PHARMACOLOGY
SO=	SO	Bibliographic Sources ^{4,5}	Word	S SO=(FERGUSON(S)J(1W)CLIN(W)PHARMACOL?)
SY=	SY	Synonyms Including Brand Names and Drug Codes ¹	Word & Phrase	S SY=INNOVACE S SY="1-(N-(S)-1-CARBOXY-3-PHENYLPROPYL"?
TC=	TC	Therapeutic Category ^{1,6}	Word	S TC=ANTIPARKINSONIAN
TN=	TN	Brand Name ¹	Phrase	S TN=EGIBREN
TV=	TV	Therapeutic Category (Veterinary) ¹	Word	S TV=(COGNITIVE(W)DISFUNCTION)
UD=	—	Update	Phrase	S UD=9999
US=	US	Uses ¹	Word	S US=(MORDANT(S)LEATHER)
UV=	UV	Ultraviolet Maximum Text ¹	Word	S UV=ALCOHOL AND UV=235
UV=	UV	Ultraviolet Maximum ^{1,7}	Numeric	S UV=260:265
DISPLAY ONLY				
—	B1	Boiling Point (Derivative)		
—	C1	CA Chemical Name (Derivative)		
—	C2	Company Name (Derivative)		
—	D1	Data Present (Derivative)		
—	D2	Relative Density (Derivative)		
—	FL	Flash Point (Derivative)		
—	L1	Lethal Dose (LD50) (Derivative)		
—	M1	Molecular Composition (Derivative)		
—	M2	Molecular Formula (Derivative)		
—	M3	Melting Point (Derivative)		
—	M4	Molecular Weight (Derivative)		
—	MC	Molecular Composition		
—	N1	Chemical Names (Derivative)		
—	N2	Chemical Names, Additional (Derivative)		
—	O1	Optical Rotation (Derivative)		
—	P1	Physical Property Information (Derivative)		
—	R1	Refractive Index (Derivative)		
—	R2	CAS Registry Number (Derivative)		
—	SB	Bibliographic Sources (Derivative)		
—	SM	Synonyms (Derivative)		
—	ST	Record Status for Retired Records		
—	T1	Brand Name (Derivative)		
—	UM	Ultraviolet Maximum (Derivative)		

⁷ Numeric values can be entered in several different ways: directly as a number, e.g. S BP=100.0; or in exponential notation, e.g. S BP=1E2. Letter abbreviations are also available: K for thousand; M for million, B for billion, e.g. S BP=0.5K:1.0K. To search a range of values, use a colon between starting and ending value, e.g. S BP=78:79 OR use numeric operators (>, <, >=, and <=), e.g. S 78<=BP<=79.

SPECIAL FEATURES

For command descriptions, enter HELP LIMIT, HELP SORT, HELP RANK, HELP MAP online.

LIMIT	/ACTIVE -- Active Records from the 14th Edition /DERIV -- Information relating to the derivative data mentioned in the monograph /MAIN -- Information relating to the main monograph substance data /RETIRED -- Records from Earlier Editions which are not being Actively Updated	S S2/ACTIVE S S2/DERIV S S1/MAIN S S1/RETIRED
SORT	MF, MN, RN, TC	SORT S2/ALL/MN PRINT S2/5/1-20/TC
RANK	All phrase- and numeric-indexed fields in the Additional Indexes can be ranked.	RANK NA RANK BP S4
MAP	MN, NA, PN, RN	MAP RN TEMP S4 MAP SYRN TEMP S3

PREDEFINED FORMAT OPTIONS

NO.	DIALOGWEB FORMAT	RECORD CONTENT
1	--	DIALOG Accession Number
2	--	Full Record, except Literature References and Physical Data
3	Medium	Full Record, except Physical Data
4	--	Full Record
5	--	Full Record
6	Free	DIALOG Accession Number/Monograph Number, Monograph Name, CAS Registry Number, and Molecular Formula
7	Long	Full Record, except Literature References
8	Short	DIALOG Accession Number/Monograph Number, Monograph Name, CAS Registry Number, Molecular Formula, Therapeutic Categories, References Present, Data Present
9	Full	Full Record
K	--	KWIC (Key Word In Context) displays a window of text; may be used alone or with other formats

OTHER OUTPUT OPTIONS

For an explanation, enter HELP TYPE, HELP UDF, HELP TAG online.

USER DEFINED FORMATS	Display codes listed in the Search Options tables can be used to customize output.	TYPE S3/MN,MF,MP,BP/1-10
TAG	Output can be displayed with tags identifying each display field.	TYPE S3/3/1-5 TAG
DIRECT RECORD ACCESS	If the accession number of a specific record is known, it can be used to display the record directly.	TYPE 03521/5 DISPLAY 03521/MN,MF,MP PRINT 03521/9

FOR ONLINE HELP:

See HELP FIELDS 304 for searchable fields; HELP FORMAT 304 for output formats; HELP LIMIT 304 for limits; HELP RATES 304 for cost information; HELP SORT 304 for sorts.