

<b>Subject Coverage</b>	Substance, toxicity, and property data for important chemicals, drugs, and agricultural and natural products		
<b>File Type</b>	Substance		
<b>Features</b>	<a href="#">CAS Registry Numbers<sup>®</sup></a> <input checked="" type="checkbox"/>	Page Images <input type="checkbox"/>	STN AnaVist <input type="checkbox"/>
	<a href="#">Keep &amp; Share</a> <input checked="" type="checkbox"/>	<a href="#">SLART</a> <input checked="" type="checkbox"/>	STN Easy <input type="checkbox"/>
	Learning Database <input type="checkbox"/>	Structures <input checked="" type="checkbox"/>	STN Viewer <input type="checkbox"/>
<b>Record Content</b>	<ul style="list-style-type: none"> <li>• Substance information such as systematic chemical names, trivial and generic names, trade names and their associated companies, CAS Registry Numbers<sup>®</sup>, molecular formulas and weights</li> <li>• Therapeutic and commercial uses</li> <li>• Structure diagrams (displayable only)</li> <li>• Bibliographic citations to the scientific and patent literature, as well as the referenced patent and other source information</li> <li>• May also contain numeric data for physical and toxicity properties</li> </ul>		
<b>File Size</b>	More than 10,600 records (02/12)		
<b>Coverage</b>	Late 19 <sup>th</sup> century-present		
<b>Updates</b>	Reloaded periodically and has no current awareness alerts		
<b>Language</b>	English		
<b>Database Producer</b>	Merck & Co., Inc. P.O. Box 2000, RY33-420 Rahway, NJ 07065-0900 USA Phone: (732) 594-7143 Fax: (732) 594-1187 E-mail: <a href="mailto:Merck_index@merck.com">Merck_index@merck.com</a>	THE MERCK INDEX ONLINE (a U.S. publication) published originally as THE MERCK INDEX <sup>®</sup> , 14th Edition (a U.S. publication) Copyright 2006, 2012 by Merck Sharp & Dohme Corp, a subsidiary of Merck & Co., Inc., Whitehouse Station, NJ, USA. All Rights Reserved.	
<b>Sources</b>	The monographs of the 14th edition of The Merck Index (a U.S. publication) and any subsequent updates. Sources include journals, books, patents, government reports, serials, symposia and conference proceedings.		
<b>User Aids</b>	<ul style="list-style-type: none"> <li>• Online Helps (HELP DIRECTORY lists all help messages available)</li> <li>• STNGUIDE</li> </ul>		
<b>Clusters</b>	<ul style="list-style-type: none"> <li>• CASRNS</li> <li>• COMPANIES</li> <li>• NUMERIC</li> </ul> <a href="#">STN Database Clusters</a> information (PDF).		
<b>Pricing</b>	See the <a href="#">STN Price List</a> or enter HELP COST at an arrow prompt (=>).		

## SEARCH and DISPLAY Field Codes

Fields that allow left truncation (/BI and /CNS) are marked with an asterisk (\*).

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index * (contains single words from the applications (APP), MERCK Index Name (MIN), CA Index Name (CN), synonyms (CN), trade names (CN), associated company names (CN), drug codes (CN), therapeutic codes (THER), therapeutic veterinary codes (VTHER), toxicity organisms (TOX), toxicity dose (TOX), toxicity route (TOX), toxicity text (TOX), notes and caution (NTE), references (RE), property data text fields, and the related fields for the derivatives, as well as molecular formulas and non-numeric terms in molecular weights and CAS Registry Numbers)	None (or /BI)	S CARDIOVAS? S 4205-90-7 S CYCLETANIDE S DRUG (L) REHAB? S BMY-28100 S ?AZEPI? S CRYSTAL# FROM ACETONITRILE S C14H12CLNO2	APP, CN, CN.DRV, Derivative, MF, MF.DRV, MIN, MW, MW.DRV, NTE, OCPP, OCPP.DRV, OTHER.DRV, <PROP>, <PROP>.DRV, RE, RE.DRV, RN, RN.DRV, THER, TOX, TOX.DRV, VTHER
Accession Number (MERCK Index Number) Application	/AN (or /MNO) /APP	S 2729/AN  S MORDANT/APP S AGRICUL? NEMATOCIDE#/APP	MNO  APP
Atom Count (1,2) CAS Registry Number	/ATC /RN (or /BI) /CN	S 6-8/ATC (L) S<=4 S 4205-90-7/RN S CEFADROXIL/CN S CEFA-DROPS/CN S CEFA?/CN (S) LENZA/CO	MF.DRV RN, RN.DRV CN, CN.DRV, MIN
Chemical Name of Derivative (contains synonyms, drug codes, and trade names for derivatives)	/CN.DRV	S VASOTEC/CN.DRV S MJ-13754-1/CN.DRV	CN.DRV
Chemical Name Segment * (2)	/CNS	S RUBROMYCIN/CNS S ?METHYLPHENYL?/CNS	CN, CN.DRV, MIN
Company Name (Corporate Name)(4) (contains corporation associated with the trade names of the parent substance and derivatives)	/CO	S BMS/CO S UNAC?/CN (S) PFIZER/CO	CN, CN.DRV
Element Count (1,2)	/ELC	S ACID (L) ELC=4 S ELC=3 (S) CL=1	Not displayed
Element Symbol (2)	/ELS	S ACID (L) ELC=4 (L) N/ELS	Not displayed
Field Availability	/FA	S L6 AND MP/FA	FA
Field Not Available	/FNA	S 215-230/MP OR MP/FNA	Not displayed
File Segment	/FS	S ACTIVE MONOGRAPHS/FS	FS
Linear Structural Formula (2)	/LSF	S AL P O4/LSF	LSF, LSF.DRV
Linear Structural Formula of Derivative	/LSF.DRV	S "(C21 H39 N7 O12"?/LSF.DRV	LSF.DRV
Material Composition (2,4,5)	/MAC	S 20-25 AL/MAC	COMP, COMP.DRV
Material Composition of Derivative (4,5)	/MAC.DRV	S 5-10 AL/MAC.DRV	COMP.DRV
MERCK Index Name	/MIN	S LIPOTROPIC HORMONE/MIN	MIN
Molecular Formula (2)	/MF	S O12S3SB2/MF S O12 S3 SB2/MF	MF, MF.DRV
Molecular Formula of Derivative	/MF.DRV	S C7H13NO2.CLH/MF.DRV S C7 H13 N O2 . CL H/MF.DRV	MF.DRV

## SEARCH and DISPLAY Field Codes (cont'd)

Search Field Name	Search Code	Search Examples	Display Codes
Molecular Weight (Formula Weight)(1,2)	/MW (or /FW)	S SALT (L) 90+-10%/MW	MW, MW.DRV
Molecular Weight of Derivative (1)	/MW.DRV	S MW.DRV<=330	MW.DRV
Notes and Caution (Warning)	/NTE (or /WARN)	S FACIAL?/NTE S FED? REG?/NTE	NTE
Number of Components (1,2)	/NC	S SULFATE (L) 2-3/NC	Not displayed
Other Sources	/OS	S CA?/OS AND L2	OS
Organism - Toxicity Test (2,4)	/ORGN	S MICE/ORGN S RAINBOW TROUT/ORGN	TOX, TOX.DRV
Organism - Toxicity Test of Derivative (4)	/ORGN.DRV	S MICE/ORGN.DRV S FEMALE RABBIT#/ORGN.DRV	TOX.DRV
Periodic Group (2)	/PG	S B7/PG;S LNTH/PG	Not displayed
Referenced Patent	/RPN	S BE553621/RPN	RPN
References (2)	/RE	S C>=23 (L) PREPN/RE S A.G. BROWN/RE S J CHROMATOGR/RE S ACE INHIBIT?/RE	RE, RE.DRV
References of Derivative	/RE.DRV	S L7 (L) PREP?/RE.DRV	RE.DRV
Route – Toxicity Test (2)	/RTE	S ORALLY/RTE	TOX, TOX.DRV
Route – Toxicity Test of Derivative	/RTE.DRV	S I.V./RTE.DRV	TOX.DRV
Specific Element Count (1,2)	/Element Symbol	S 5/NA	Not displayed
Therapeutic Codes	/THER	S ANTIDEPRESSANT/THER S ADRENERGIC BLOCKER/THER	THER
Toxicity Text (contains organism, route, dose, and text) (2)	/TOX	S RAT#/TOX	TOX, TOX.DRV
Toxicity Text of Derivative	/TOX.DRV	S DUCKLING#/TOX.DRV	TOX.DRV
Type of Derivative	/TYP.DRV	S CALCIUM SALT?/TYP.DRV	DERIVATIVE
Veterinary Therapeutic Codes	/VTHER	S ANTICOAGULANT/VTHER	VTHER

(1) Numeric search field that may be searched with numeric operators or ranges.

(2) Includes derivatives.

(3) There is currently no data in this search field.

(4) Search with implied (S) proximity is available in this field.

(5) Combination numeric and text field. The percent composition terms are numeric and may be searched using numeric operators or ranges. The Alloy component terms are text terms.

## Property Search and Display Field Codes

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Boiling Point (1,2) Pressure (1,2)	deg C mm Hg	/BP /BP.P	S NITRILE AND 14+-5%/BP S 2-8 PSI/BP.P S 230-235/BP (P) 120-130/BP.P	BP, BP.DRV BP, BP.DRV
Boiling Point of Derivative (1) Pressure Lethal Dose at 50% (1,2)	deg C mm Hg none	/BP.DRV /BP.P.DRV /LD50	S 68-80/BP.DRV S BP.P.DRV<0.50 S .35-.50/LD50 S .35-.50/LD50 (P) I.P./RTE	BP.DRV BP.DRV BP.DRV
Lethal Dose at 50% of Derivative (1) Melting Point (1,2) Melting Point of Derivative (1) Optical Rotatory Power (1,2) Spectral Line (2)	none deg C deg C deg -	/LD50.DRV /MP /MP.DRV /ORP /ORP.SL	S LD50.DRV>=89 S RESIN# AND 250-275/MP S 225+-3% K/MP.DRV S 75.6+-5%/ORP S 589NM/ORP.SL S 589/ORP.SL	TOX, TOX.DRV TOX.DRV MP, MP.DRV MP.DRV ORP, ORP.DRV ORP, ORP.DRV
Temperature (1,2) Optical Rotatory Power of Derivative (1) Spectral Line Temperature (1)	deg C deg - deg C	/ORP.T /ORP.DRV /ORP.SL.DRV /ORP.T.DRV	S 15-25/ORP.T S OIL# AND ORP.DRV=48+-10 S 365/ORP.SL.DRV S 15-25/ORP(P)15-25/ORP.T.DRV	ORP, ORP.DRV ORP.DRV ORP.DRV ORP.DRV
Refractive Index (1,2) Spectral Line (2) Temperature (1,2) Refractive Index of Derivative (1) Spectral Line Temperature (1) Specific Gravity (1,2)	none - deg C none - deg C none	/RI /RI.SL /RI.T /RI.DRV /RI.SL.DRV /RI.T.DRV /SPGR	S 1.37+-5%/RI OR RI/FNA S D/RI.SL S RI.T=20 AND LIQUID S RI.DRV>1.48 (P) RI.T.DRV=20 S D/RI.SL.DRV S 68 F/RI.T.DRV S .82-.92/SPGR	RI, RI.DRV RI, RI.DRV RI, RI.DRV RI.DRV RI.DRV RI.DRV SPGR, SPGR.DRV
Reference Temperature (1,2)	deg C	/SPGR.RT	S 298.15K/SPGR.RT	SPGR, SPGR.DRV
Temperature (1,2)	deg C	/SPGR.T	S 57-62/SPGR.T	SPGR, SPGR.DRV
Specific Gravity of Derivative (1) Reference Temperature (1)	none deg C	/SPGR.DRV /SPGR.RT.DRV	S SPGR.DRV<=1.854 S SPGR.RT.DRV>90	SPGR.DRV SPGR.DRV
Temperature (1)	deg C	/SPGR.T.DRV	S SPGR.DRV<=1.854 (P) SPGR.T.DRV<=60	SPGR.DRV
Toxicity Dose (1,2) Toxicity Dose of Derivative (1) UV and Visible Spectrum Peak Position (1,2) UV and Visible Spectrum Peak Position of Derivative (1)	none none nm nm	/DOSE /DOSE.DRV /UVS.PP /UVS.PP.DRV	S 0.5-0.6/DOSE (L) ORAL?/RTE S 25-30/DOSE.DRV (P) MICE S CRYSTAL? AND UVS.PP>=90 S 240+-10/UVS.PP.DRV	TOX, TOX.DRV TOX.DRV UVS, UVS.DRV UVS.DRV

(1) Numeric search field that may be searched with numeric operators or ranges.

(2) Includes the derivatives.

(3) There is currently no data in this search field.

## DISPLAY and PRINT Formats

Any combination of formats may be used to display or print answers. Multiple codes must be separated by commas or spaces, e.g., D L1 1-5 CN RN. The fields are displayed or printed in the order requested. When more than one derivative is contained in the record, each derivative and its associated information is displayed.

Hit-term highlighting is available in the APP, CN, CN.DRV, COMP, COMP.DRV, LSF, LSF.DRV, MF, MF.DRV, MIN, MNO, MW, MW.DRV, NTE, OCPP, OCPP.DRV, OS, OTHER.DRV, RE, RE.DRV, RN, RN.DRV, RPN, THER, TOX, TOX.DRV, and VOTHER. Highlighting must be ON during SEARCH in order to use the HIT, KWIC, and OCC formats.

Format	Content	Examples
APP	Application	D L1 3 APP
BP	Boiling Point of Parent Substance	D BP 1,3-5
BP.DRV	Boiling Point of Derivative	D BP.DRV 5-10
CN	Chemical Name of Parent Substance (includes MERCK Index Name, CA Index Name, Synonyms, Drug Codes, and Trade Names and associated corporations)	D 1-3,7,8 CN
CN.DRV	Chemical Name of Derivative	D CN.DRV
COMP	Composition of Parent Substance	D COMP
COMP.DRV	Composition of Derivative	D COMP.DRV 1-5
FA (1)	Field Availability	D L1 FA 3
FS	File Segment	D FS
LSF	Linear Structural Formula of Parent Substance	D 1,3,6 LSF L5
LSF.DRV	Linear Structural Formula of Derivative	D LSF.DRV
MF	Molecular Formula of Parent Substance	D 1,4 MF
MF.DRV	Molecular Formula of Derivative	D L1 MF.DRV
MIN (1)	MERCK Index Name	D MIN
MNO (AN)	MERCK Index Number (Accession Number)	D L4 1-4 AN
MP	Melting Point of Parent Substance	D MP L1 4
MP.DRV	Melting Point of Derivative	D MP.DRV 3,4
MW (FW)	Molecular Weight (Formula Weight) of Parent Substance	D MW
MW.DRV	Molecular Weight Derivative	D MW.DRV
NTE (WARN)	Notes and Caution	D NTE
OCPP	Other Chemical/Physical Properties of Parent Substance	D OCPP 2 L5
OCPP.DRV	Other Chemical/Physical Properties of Derivative	D OCPP.DRV 2
ORP	Optical Rotatory Power of Parent Substance	D L3 4 ORP
ORP.DRV	Optical Rotatory Power of Derivative	D ORP.DRV
OS	Other Source	D OS
OTHER.DRV	Other Information Regarding Derivatives	D 5,3 OTHER.DRV
RE	References of Parent Substance	D RE
RE.DRV	References of Derivative	D L4 RE.DRV 3
RI	Refractive Index of Parent Substance	D L3 2 RI
RI.DRV	Refractive Index of Derivative	D RI.DRV
RN	CAS Registry Number of Parent Substance	D 1-3,5 RN L3
RN.DRV	CAS Registry Number of Derivative	D RN.DRV
RPN	Referenced Patent	D RPN 1-10
SPGR	Specific Gravity of Parent Substance	D L2 SPGR 3,4-7
SPGR.DRV	Specific Gravity of Derivative	D SPGR.DRV
STF (2)	Flat Structure (no stereo indicated)	D L9 1 3 STF
STF.DRV (2)	TYP.DRV, Flat Structure of Derivative	D STF.DRV
STR (3)	Structure Diagram (includes stereo bonds and R/S/E/Z labels when available)	D L4 STR
STR.DRV (3)	TYP.DRV, Structure Diagram of Derivative (includes stereo bonds and R/S/E/Z labels when available)	D L4 STR.DRV
STS (2,3)	Stereo Structure (includes stereo bonds when available)	D STS
STS.DRV (2,3)	TYP.DRV, Stereo Structure of Derivative (includes stereo bonds when available)	D STS.DRV
THER	Therapeutic Codes	D THER
TOX	Toxicity Text	D TOX 1-5
TOX.DRV	Toxicity Text Derivative	D L4 TOX.DRV
TYP.DRV (1)	Type of Derivative	D TYP.DRV

**DISPLAY and PRINT Formats (cont'd)**

Format	Content	Examples
UVS	UV and Visible Spectrum of Parent Substance	D UVS 1-4
UVS.DRV	UV and Visible Spectrum Derivative	D UVS.DRV 2 L4
VOTHER	Therapeutic Codes - Veterinary	D L7 VOTHER
ALL (3)	MNO, RN, MIN, CN, FS, MF, LSF, COMP, MW, RE, STR, BP, MP, RI, ORP, SPGR, TOX, UVS, OCPP, TYP.DRV, RN.DRV, CN.DRV, MF.DRV, LSF.DRV, COMP.DRV, MW.DRV, STR.DRV, RE.DRV, BP.DRV, MP.DRV, RI.DRV, ORP.DRV, SPGR.DRV, TOX.DRV, UVS.DRV, OCPP.DRV, OTHER.DRV, NTE, APP, THER, VOTHER, OS, RPN	D 2 ALL L4
DRV (3)	TYP.DRV, RN.DRV, CN.DRV, MF.DRV, LSF.DRV, COMP.DRV, MW.DRV, RE.DRV, STR.DRV, BP.DRV, MP.DRV, RI.DRV, ORP.DRV, SPGR.DRV, TOX.DRV, UVS.DRV, OCPP.DRV, OTHER.DRV	D 1 3 DRV
IDE (3)	MNO, RN, MIN, CN, FS, MF, LSF, COMP, MW, STR	D 3-5 L2 IDE
IDETAB	Table containing MNO, MIN, RN, and MF for a single answer or several records in a single table	D L4 IDETAB 1-3
IDE.DRV	Table containing TYP.DRV, CN.DRV, RN.DRV, and MF.DRV for each derivative of a single answer	D IDE.DRV 6
MONO (3)	MNO, RN, MIN, CN, FS, MF, LSF, COMP, MW, RE, STR, OCPP, TYP.DRV, RN.DRV, CN.DRV, MF.DRV, LSF.DRV, COMP.DRV, MW.DRV, RE.DRV, STR.DRV, OCPP.DRV, OTHER.DRV, NTE, APP, THER, VOTHER	D MONO
PHYS	BP, MP, RI, ORP, SPGR, TOX, UVS, OCPP (QRD is the default)	D PHYS D QRD L8
QRD	Query Related Data (MNO, RN, MIN and all fields containing the hit terms)	
SAM (1)	MNO, RN, MIN, MF, FA	D SAM TOTAL
SCAN (1,4)	CN (MIN only), RN (random display without answer numbers)	D SCAN
HIT	Fields containing hit terms	D HIT 5,3
KWIC	Hit terms with 20 words on either side (KeyWord-In-Context)	D KWIC NOH
OCC (1)	Fields that contain hit terms and number of times they occur	D 1-3,5-6 OCC

(1) No online display fee for this format.

(2) Custom display only.

(3) Stereo structure diagrams are available only on graphics terminals and in offline prints, or when using STN Express with *Discover!* Or STN on the Web. When a structure is displayed on a text terminal, STF is displayed.

(4) SCAN must be specified on the command line, e.g., D SCAN.

## SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphabetic or numeric order of the specified field(s).

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT (2)
Accession Number	AN	N	Y
Application	APP	Y	N
Boiling Point of Derivative	BP.DRV	N	Y
Boiling Point of Parent	BP	N	Y
CAS Registry Number and Chemical Names of Parent	CHEM	Y (3,4)	N
CAS Registry Number of Derivative	RN.DRV	Y (5)	N
CAS Registry Number of Parent	RN	Y (5)	N
Chemical Name of Derivative	CN.DRV	Y (6)	N
Chemical Name of Parent	CN	Y (7)	N
	NAME	Y (8)	N
Company Name of Derivative	CO.DRV	Y	N
Company Name of Parent	CO	Y	N
File Segment	FS	Y	N
Formula Weight of Parent	FW	N	Y
Linear Structural Formula of Derivative	LSF.DRV	Y (9)	N
Linear Structural Formula of Parent	LSF	Y	N
Melting Point of Derivative	MP.DRV	N	Y
Melting Point of Parent	MP	N	Y
MERCK Index Name	MIN	Y	Y
MERCK Index Number	MNO	N	Y
Molecular Formula of Derivative	MF.DRV	Y (10)	N
Molecular Formula of Parent	MF	Y (default)	N
Molecular Weight of Derivative	MW.DRV	N	Y
Molecular Weight of Parent	MW	N	Y
Note and Cautions	NTE	Y	N
Occurrence Count of Hit Terms	OCC	N	Y
Optical Rotatory Power of Derivative	ORP.DRV	N	Y
Optical Rotatory Power of Parent	ORP	N	Y
Other Chemical/Physical Properties of Derivative	OCPP.DRV	Y (5)	N
Other Chemical/Physical Properties of Parent	OCPP	Y (5)	N
Other Information Regarding Derivatives	OTHER.DRV	Y (5)	N
Other Sources	OS	Y	N
Referenced Patents	RPN	Y	N
References of Derivative	RE.DRV	Y (11)	N
References of Parent	RE	Y	N
Refractive Index of Derivative	RI.DRV	N	Y
Refractive Index of Parent	RI	N	Y
Specific Gravity of Derivative	SPGR.DRV	N	Y
Specific Gravity of Parent	SPGR	N	Y
Therapeutic Codes	THER	Y	N
Therapeutic Codes, Veterinary	VTHER	Y	N
Type of Derivative	TYP.DRV	Y (5,12)	N

- (1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answer set, e.g., SEL HIT CN. However, when the term is searched in a field that searches both the parent and derivatives, SEL HIT must be used with the corresponding field. For example, if the chemical name is searched in /CN and the hit is in the derivative information, SEL HIT CN does not generate an extracted term. SEL HIT CN.DRV would generate an extracted term.
- (2) For fields that contain more than one value, SORT is performed on the first value listed.
- (3) Selects or analyzes the CAS Registry Number and the MERCK Index Name, CA Index Name, Synonyms, Drug Codes, and Trade Names and appends /BI to the terms created by SELECT.
- (4) SELECT HIT and ANALYZE HIT are not valid if the hit term is a Trade Name.
- (5) Appends /BI to the terms created by SELECT.

**MRCK****SELECT, ANALYZE, and SORT Fields (cont'd)**

- (6) Selects or analyzes CA Index Name, Synonyms, Drug Codes, and Trade Names of the derivatives and appends /CN to the terms created by SELECT.
- (7) Selects or analyzes the MERCK Index Name, CA Index Name, Synonyms, Drug Codes, and Trade Names and appends /CN to the terms created by SELECT.
- (8) Selects or analyzes the MERCK Index Name, CA Index Name, Synonyms, Drug Codes, and Trade Names and appends /BI to the terms created by SELECT.
- (9) Appends /LSF to the terms created by SELECT.
- (10) Appends /MF to the terms created by SELECT.
- (11) Appends /RE to the terms created by SELECT.
- (12) SELECT HIT and ANALYZE HIT are not valid with this field.

**Sample Records****DISPLAY ALL**

COPYRIGHT (C) 2006, 2012 Merck Sharp and Dohme

Corp., a subsidiary of Merck and Co., Inc., Whitehouse Station, N.J.,

U.S.A. All rights reserved. on STN

MERCK Number (MNO): 1402403

CAS Registry No. (RN): 23887-31-2

MERCK Index Name (MIN): Clorazepic Acid

CA Index Name (CN): 7-Chloro-2,3-dihydro-2-oxo-5-phenyl-1H-1,4-benzodiazepine-3-carboxylic acid

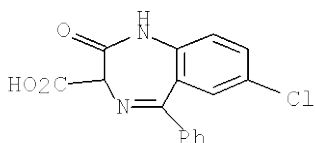
File Segment. (FS): Active Monographs

Molecular Form. (MF): C16 H11 Cl N2 O3

Wgt Composition (COMP): C 61.06%, H 3.52%, Cl 11.26%, N 8.90%, O 15.25%.

Molecular Weight (MW): 314.72

References (RE): Prepn: NL 6507637; J. Schmitt, US 3516988; reissued as US RE 28315 (1965, 1970, 1975 all to Clin-Byla). Synthesis and activity of the dipotassium salt: J. Schmitt et al., Chim. Ther. 4, 239 (1969). Solution chemistry: R. Raveux, M. Briot, ibid. 303. Metabolism: P. Gros, R. Raveux, ibid. 312. Toxicity data: M. Brunaud et al., Arzneim.-Forsch. 20, 123 (1970). Series of articles on pharmacology and clinical use: ibid. 123-137. HPLC determn in plasma: P. Colin, G. Sirois, J. Chromatogr. 273, 367 (1983). Clinical trial in anxiety: W. W. K. Zung, J. Clin. Psychiatry 48, 13 (1987); in comparison with buspirone (MRCK 1401504), q.v.: K. Rickels et al., Arch. Gen. Psychiatry 45, 444 (1988). Comprehensive description: J. A. Raihle, V. E. Papendick, Anal. Profiles Drug Subs. 4, 91-112 (1975).



== DERIVATIVE == (1): Dipotassium salt

CAS Registry No. (RN.DRV): 57109-90-7

CA Index Name (CN.DRV): 7-Chloro-2,3-dihydro-2-oxo-5-phenyl-1H-1,4-benzodiazepine-3-carboxylic acid monopotassium salt compd with potassium hydroxide

Synonym(s) (CN.DRV): Clorazepate dipotassium

Drug Code(s) (CN.DRV): Abbott 35616; CB-4306

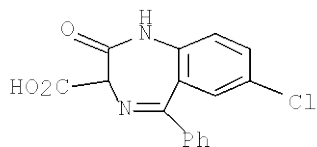
Trade Name(s) (CN.DRV): Belseren (Bristol-Myers Squibb Co.; BMS); Mendon (Dainippon Pharmaceutical Co., Ltd.; Dainippon); Tranxilene (Clin-Comar-Byla); Tranxilium (Heinrich Mack Nachf., Gmbh & Co. KG (subsidiary of Pfizer Inc.); Mack, Illert.); Transene (Clin-Comar-Byla); Tranxene (Abbott Labs.; Abbott)

Molecular Form. (MF.DRV): C16 H11 Cl K2 N2 O4

Wgt Composition (COMP.DRV): C 46.99%, H 2.71%, Cl 8.67%, K 19.12%, N 6.85%, O 15.65%.

Molecular Weight (MW.DRV): 408.92

CM 1



● K

CM 2

K-OH

Toxicity (TOX.DRV):

LD50 in mice (mg/kg): 700 orally; 290 i.p. LD50 orally in rats: &gt;1000 mg/kg (Brunaud).

UV Spectrum (UVS.DRV):

Part 1 of 2	Deriv. Number	Derivative Type
1	1	Dipotassium salt
2		
3		

UV Spectrum (UVS.DRV):

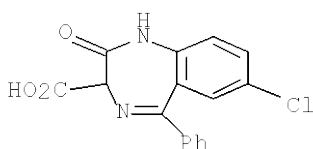
Part 2 of 2	Maximum Peak Pos. UVS.PP.DRV nm	Note
1	231	(anhydrous product in water) ( $\epsilon$ 33500,
2		2450)
3	311	

**MRCK**

## Other Properties (OCPP.DRV):

White powder, freely sol in water. Very poorly sol in ethanol.  
 Practically insol in ether, chloroform. Aq solns are alkaline to  
 phenolphthalein. uv max (anhydrous product in water): 231 , 311 nm  
 (ε 33500, 2450) . LD50 in mice ( mg/kg ): 700 orally ; 290  
 i.p. LD50 orally in rats: > 1000 mg/kg (Brunaud) .

== DERIVATIVE == (2): Monopotassium salt  
 CAS Registry No. (RN.DRV): 5991-71-9  
 Drug Code(s) (CN.DRV): CB-4311  
 Trade Name(s) (CN.DRV): Azene (Endo Pharmaceuticals, Inc.; Endo)  
 Molecular Form. (MF.DRV): C16 H10 Cl K N2 O4  
 Wgt Composition (COMP.DRV): C 52.11%, H 2.73%, Cl 9.61%, K 10.60%, N 7.60%, O  
 17.35%.  
 Molecular Weight (MW.DRV): 368.81



## Notes (NTE):

Note: This is a controlled substance (depressant): 21 CFR, 1308.14.

## Therapeutic Codes (THER):

Anxiolytic.; Anxiolytic; Benzodiazepine Derivatives

## Referenced Patent (RPN):

NL6507637; US3516988; US28315

**In North America**

CAS  
 STN North America  
 P.O. Box 3012  
 Columbus, Ohio 43210-0012 U.S.A.

CAS Customer Center:  
 Phone: 800-753-4227 (North America)  
 614-447-3700 (worldwide)  
 Fax: 614-447-3751  
 E-mail: help@cas.org  
 Internet: www.cas.org

**In Europe**

FIZ Karlsruhe  
 STN Europe  
 P.O. Box 2465  
 76012 Karlsruhe  
 Germany  
 Phone: +49-7247-808-555  
 Fax: +49-7247-808-259  
 E-mail: helpdesk@fiz-karlsruhe.de  
 Internet: www.stn-international.com

**In Japan**

JAICI (Japan Association for  
 International Chemical Information)  
 STN Japan  
 Nakai Building  
 6-25-4 Honkomagome, Bunkyo-ku  
 Tokyo 113-0021, Japan  
 Phone: +81-3-5978-3601 (Technical Service)  
 +81-3-5978-3621 (Customer Service)  
 Fax: +81-3-5978-3600  
 E-mail: support@jaici.or.jp (Technical Service)  
 customer@jaici.or.jp (Customer Service)  
 Internet: www.jaici.or.jp