

## Chapman and Hall Chemical Database

### FILE DESCRIPTION

The **Chapman & Hall Chemical Database** (CHCD), formerly HEILBRON, the chemical properties database, represents the complete text of several chemical dictionaries from Chapman and Hall. CHCD is a source database of chemical identification, physical-chemical properties, use, hazard, and key reference data to the world's more important chemical substances, as selected by a panel of experts. CHCD provides chemical substance identification through searching physical and/or chemical properties, compound variants, derivative names, synonyms, CAS® Registry numbers, molecular formulae and molecular weight, biological source statements, use/importance data, melting point, freezing point, boiling point, solubility, relative density, optical rotation, and dissociation constants, as well as providing suppliers and toxicity data.

### SUBJECT COVERAGE

- Fundamental acyclic, alicyclic, aromatic and heterocyclic organic compounds.
- Comprehensive coverage for natural products including alkaloids, amino acids, antibiotics, carbohydrates, flavonoids, lichen acids, lignans, nucleosides, peptides, steroids, tannins, and terpenoids.
- Pharmaceuticals including marketed drugs and compounds in clinical trials.
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- Analytical reagents: biological status, extractants, indicators, nmr shift reagents, resolving agents.
- Industrial chemicals, synthetic reagents and laboratory solvents.
- A wide range of inorganic and organometallic compounds, covering coordination complexes and cluster compounds.
- Compounds with unusual structural, physical or chemical properties.

### SOURCES

CHCD is the online version of the database used to produce the *Dictionary of Organic Compounds - 5th Edition*, (DOC 5) and the *Dictionary of Organometallic Compounds* (DMC) and supplements. The contents of the database are prepared from the primary and secondary chemical literature under the supervision of a panel of subject experts. Material from the following source books is also included: *Carbohydrates*, *Amino Acids and Peptides*, the *Dictionary of Antibiotics and Related Compounds*, and the *Dictionary of Organophosphorus Compounds*.

### DIALOG FILE DATA

Inclusive Dates:

Latest editions of printed counterparts (which include citations from chemical literature to the present, with many pre-1967 citations)

Update Frequency: Irregular

File Size: 442,257 records as of May 1997

### CONTACT

The Chapman and Hall Chemical Database is produced by Chapman & Hall/ CRC (UK). Questions concerning file content should be directed to:

Dr. Fiona Macdonald

Managing Editor, Chapman & Hall/CRC

23 Blades Court, Deodar Road

London SW15 2NU

United Kingdom

Phone: +44 (0) 208 875 4375

Fax: +44 (0) 208 871 3443

E-Mail: fmacdonald@crcpress.com

## FORMAT 5 AND 9 FULL RECORD

DIALOG(R)File 303:Chapman & Hall Chemical Database  
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/MAIN 00007992  
 SF= Subfile: Dictionary of Natural Products, 1994  
 CHCD Acc. No: A-01440V0  
 AA= Unique Key: 00019586- -00  
 /NA, NA=, /DE, /CN, CN= CHCD NAME: 4-Amino-3-isoxazolidinone  
 /SY, SY=, /DE, /NA, NA= Synonyms: Cycloserine ; Cyclomycin; Closina; Micoserina;  
 Farmiserina; Orientomycin; Oxymycin; Antibiotic 106-7;  
 Antibiotic 5915; Antibiotic 8217; Antibiotic 17452;  
 Antibiotic E 733A; Antibiotic I 1431; Antibiotic K 300;  
 Antibiotic NJ 21; Antibiotic PA 94;  
 /TX Compound Type: Drug - Antibacterial agents; Drugs - Antibiotics;  
 Drugs - Tuberculostatic agents  
 RN= CAS Registry No: 4834-58-6  
 Additional CAS Reg. No: 339-72-0  
 MF= Molecular Formula: C3H6N2O2  
 MW= Molecular Wt: 102.093  
 Unique Key: 00019586-A-00  
 /VAR VARIANT: 4-Amino-3-isoxazolidinone\ (R)-form  
 Compound Type: Selected General Organics - Miscellaneous  
 modified aminoacids; Natural Products - Miscellaneous  
 modified aminoacids; Natural Products - Isoazole alkaloids  
 Hazard: CNS adverse effects reported when used  
 therapeutically. LD50 (mus, orl) 5290 mg/kg  
 Source: Prod. by Streptomyces garyphalus, Streptomyces  
 orchidaceus, Streptomyces lavendulae and Streptomyces  
 nagasakiensis  
 Use/Importance: Shows antibiotic activity primarily against  
 mycobacteria.  
 Tuberculostatic  
 Physical State: Cryst.  
 Miscellaneous: Of limited clinical use due to toxicity  
 CAS Registry No: 68-41-7  
 RTECS No.: NY2975000  
 Solubility: Sol. H2O, alkalis  
 Optical Rotation: +116 deg at 23 deg C (c, 1.17 in H2O)  
 wavelength Na line  
 Melting Pt: Mp 155-156 deg C (dec.)  
 Unique Key: 00019586-A-01  
 /DERIV DERIVATIVE: 4-Amino-3-isoxazolidinone\ (R)-form\ N-Ac  
 Physical State: Needles  
 Molecular Formula: C5H8N2O3  
 Molecular Wt: 144.130  
 Melting Pt: Mp 179-180 deg C  
 Unique Key: 00019586-A-02  
 /DERIV DERIVATIVE: 4-Amino-3-isoxazolidinone\ (R)-form\ N N'-Di-Ac  
 Physical State: Chunky needles (Me2CO)  
 Molecular Formula: C7H10N2O4  
 Molecular Wt: 186.167  
 Melting Pt: Mp 121-122 deg C  
 Unique Key: 00019586-B-00  
 /VAR VARIANT: 4-Amino-3-isoxazolidinone\ (S)-form  
 CAS Registry No: 339-72-0  
 Optical Rotation: -104 deg at 20 deg C (c, 1 in H2O)  
 wavelength Na line  
 Melting Pt: Mp 146 deg C (dec.)  
 Unique Key: 00019586-C-00  
 /VAR VARIANT: 4-Amino-3-isoxazolidinone\ (+/-)-form  
 CAS Registry No: 68-39-3  
 RTECS No.: NY2974900  
 Melting Pt: Mp 137-140 deg C  
 References:  
 01 Aldrich Library of FT-IR Spectra, 1st edn. 810A (ir)  
 02 Aldrich Library of NMR Spectra, 2nd edn. 1 678B (nmr)  
 03 Harned RL et al., Antibiot. Chemother. (Washington, D.C.)  
 1955 5 204 (struct)  
 04A Stammer CH et al., J.A.C.S. 1955 77 2344, 2345, 2346  
 04B 1957 79 3236 (struct, synth, isol, resoln)  
 05 Neuhaus FC Antibiotics (N.Y.) 1967 1 40 (rev)  
 06 Milne GWA et al., Tetrahedron 1967 23 65 (nmr, ms)  
 07 Lamb JW Anal. Profiles Drug Subst. 1972 1 53 (rev, synth,  
 anal)

## FORMAT 5 AND 9 FULL RECORD (cont'd)

08 O'Brien P Met. Ions Biol. Syst. 1985 19 295 (rev, pharmacol)  
 09 Negwer M Organic-Chemical Drugs and their Synonyms  
 6th Ed., Akademie-Verlag, Berlin 1987 107 (synonyms)  
 10 El-Obeid HA et al., Anal. Profiles Drug Subst. 1989 18 567  
 (rev)  
 11 Merck Index 11th edn. 1989 2758  
 12 Martindale, The Extra Pharmacopoeia 30th edn.,  
 Pharmaceutical Press, London 1993 156  
 79 Lewis RJ Sax's Dangerous Properties of Industrial  
 Materials  
 8th Ed., Van Nostrand-Reinhold 1992 CQH000

**/DP, DP=** Data Tags: Cas Registry number; Molecular formula; Compound  
 Variants; Source; Use/Importance; Physical State; Solubility;  
 Melting Point; Optical Rotation; Miscellaneous Data;  
 Hazard/Toxicity Data; Rtecs Reference; Derivatives

## FORMAT 2, 3, 4 AND 7 INDIVIDUAL COMPOUND

DIALOG(R)File 303:Chapman & Hall Chemical Database  
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**/VAR** 00007993  
**SF=** Subfile: Dictionary of Natural Products 1994  
**AA=** Unique key: 00019586-A-00  
**/NA, NA=, /CN** VARIANT: 4-Amino-3-isoxazolidinone\ (R)-form  
**RN=** CAS Registry No: 68-41-7  
**/TX** Compound Type: Selected General Organics - Miscellaneous  
 modified aminoacids Natural Products - Miscellaneous  
 modified aminoacids Natural Products - Isoazole alkaloids

**RR=** RTECS: NY2975000  
**/TX** Hazard: CNS adverse effects reported when used therapeutically.  
 LD50 (mus, orl) 5290 mg/kg

**/TX** Source: Prod. by Streptomyces garyphalus, Streptomyces  
 orchidaceus, Streptomyces lavendulae and Streptomyces  
 nagasakiensis

**/TX** Use/Importance: Shows antibiotic activity primarily against  
 mycobacteria.  
 Tuberculostatic

**PS=** Physical State: Cryst.  
**MP=** Melting Pt.: Mp 155-156 deg C (dec.)  
**SL=** Solubility: Sol. H2O, alkalis  
**OP=, OT=** Optical Rotation: +116 deg at 23 deg C (c, 1.17 in H2O)  
 wavelength Na line

**/TX** Miscellaneous: Of limited clinical use due to toxicity  
**/DP, DP=** Data Tags: Compound Variants; Cas Registry number; Source;  
 Use/Importance; Physical State; Solubility; Melting Point; Optical  
 Rotation; Miscellaneous Data; Hazard/Toxicity Data; Rtecs Reference

**Note: /MAIN, /DERIV, and /VAR search only the individual compound**

## SEARCH OPTIONS

## BASIC INDEX

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
— /CN	— CN	All Basic Index Fields Main CHCD Substance Name, Variant Name(s), Derivative Name(s) <sup>1,2,4</sup>	Word Segment & Word & Phrase	S AMINO(1W)ISOXAZOLIDINONE S ONE/CN S AMINO(1W)ISOXAZOLIDINONE/CN S 4-AMINO-3-ISOXAZOLIDINONE/CN
/DE	DE	CHCD Name, Variant Name, Derivative Name, and Synonyms <sup>1,2,4,5</sup>	Segment & Word & Phrase	S ONE/DE S AMINO(1W)ISOXAZOLIDINONE/DE S 4-AMINO-3-ISOXAZOLIDINONE/DE
/DERIV	—	Derivative Substance Information <sup>4</sup>	Segment & Word & Phrase	S ONE/DERIV S AMINO(1W)ISOXAZOLIDINONE/NA,DERIV S 4-AMINO-3-ISOXAZOLIDINONE?/DERIV
/DP	DP	Data Present <sup>1,4</sup>	Word & Phrase	S BOILING(W)POINT/DP S BOILING POINT/DP
/EC	—	Element Count <sup>4</sup>	Word	S C3/EC
/MAIN	—	Main CHCD Substance Information <sup>4</sup>	Segment & Word & Phrase	S ONE/MAIN S AMINO(1W)ISOXAZOLIDINONE/MAIN,NA S 3-AMINO-3-ISOXAZOLIDINONE/MAIN
/NA	NA	CHCD Name, Variant Name, Derivative Name, and Synonyms <sup>1,2,4</sup>	Segment & Word & Phrase	S ONE/NA S AMINO(1W)ISOXAZOLIDINONE/NA S 4-AMINO-3-ISOXAZOLIDINONE/NA
/SY	SY	Synonyms <sup>1,2,4</sup>	Segment & Word & Phrase	S CYCLO/SY S ANTIBIOTIC(W)17452/SY S ANTIBIOTIC 17452/SY
/TX	TX	Text <sup>3,4</sup>	Word	S CNS(W)ADVERSE/TX
/VAR	—	Compound Variant Information <sup>4</sup>	Segment & Word & Phrase	S ONE/VAR S (ISOAZOLE(W)ALKALOIDS)/VAR,NA S 4-AMINO-3-ISOXAZOLIDINONE?/VAR

<sup>1</sup> Searchable in the Basic Index and in the Additional Indexes.

<sup>2</sup> 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.

<sup>3</sup> The Text field includes Compound Type, Hazard Information, General Information, Source of Substance, Use/Importance, Miscellaneous, and Physical State.

<sup>4</sup> Terms can be qualified to any one of three levels using one of the following suffixes: /MAIN to restrict retrieval to the Main CHC substance information; /VAR to restrict retrieval to the Compound Variant substance information, and /DERIV to restrict retrieval to the Derivative substance information (e.g., MP=24/VAR retrieves compound variant substances with a melting point of 24).

<sup>5</sup> Also /DF.

## ADDITIONAL INDEXES

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
AA=	AA	Unique ID	Phrase	S AA=00019586-A-00
—	AN	DIALOG Accession Number		
BP=	BP	Boiling Point (degrees Celsius) <sup>4,6</sup>	Numeric	S BP=120
BT=	BP	Boiling Point Text <sup>4</sup>	Word	S BT=2MM(F)BP=120
CN=	CN	Main CHCD Substance Information <sup>1,4</sup>	Phrase	S CN=4-AMINO-3-ISOXAZOLIDINONE
DP=	DP	Data Present	Phrase	S DP=BOILING POINT
EC=	—	Element Count <sup>4</sup>	Word	S EC=C0003
ME=	MF	Molecular Element <sup>4</sup>	Phrase	S ME=CHNO
MF=	MF	Molecular Formula <sup>4</sup>	Phrase	S MF=C3H6N2O2 S MF=C3H6N2O2/MAIN S MF=C5H8N2O3/DERIV S MF=C13H9NO/VAR
MP=	MP	Melting Point (degrees Celsius) <sup>4,6</sup>	Numeric	S MP=155
MW=	MW	Molecular Weight <sup>4,6</sup>	Numeric	S MW=102.093
NA=	NA	Chemical Name <sup>1,4</sup>	Phrase	S NA=CYCLOSERINE
OP=	OP	Optical Rotation (degrees) <sup>4,6</sup>	Numeric	S OP=116
OT=	OP	Optical Rotation Text <sup>4</sup>	Word	S OT=(NA(W)LINE)
PK=	PK	Dissociation Constant (pKa) <sup>4,6</sup>	Numeric	S PK=9.47
PS=	PS	Physical State <sup>4</sup>	Word	S PS=CRYST?
RN=	RN	CAS(R) Registry Number <sup>4</sup>	Phrase	S RN=4834-58-6 S RN=339-72-0/VAR S RN=23113-01-1/DERIV
RR=	RR	RTECS Reference <sup>4</sup>	Phrase	S RR=NY2975000
SF=	SF	Dictionary Name (Subfile)	Phrase	S SF=DICTIONARY OF NATURAL PRODUCTS
SG=	SG	Specific Gravity or Relative Density <sup>4,6</sup>	Numeric	S SG=1.10:1.25
SL=	SL	Solubility <sup>4</sup>	Word	S SL=(SOL(2W)ALKALIS)
ST=	SG	Specific Gravity Text	Word	S ST=(AT(W)20(W)DEG(W)C)
UD=	—	Update	Phrase	S UD=9999

<sup>6</sup> Numeric values can be entered in several different ways: directly as a number, i.e., S BP=100.0; in exponential notation, i.e., 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.

<b>LIMIT</b>	/DOC -- Dictionary of Organic Compounds /HZ -- Hazard/Toxicity Data available /NOHZ -- Hazard/Toxicity Data unavailable	S S3/DOC S S4/HZ S S2/NOHZ
<b>SORT</b>	AA, MF, RN	SORT S1/ALL/RN,D PRINT S5/5/1-24/MF
<b>RANK</b>	All phrase- and numeric-indexed fields in the Additional Indexes can be ranked.	RANK NA RANK SF S4
<b>MAP</b>	RN, SY	MAP RN TEMP S2

**PREDEFINED FORMAT OPTIONS**

NO.	DIALOGWEB FORMAT	RECORD CONTENT
1	--	DIALOG Accession Number
2	--	Individual Compound (Variant, Derivative, or Main Compound)
3	Medium	Individual Compound (Variant, Derivative, or Main Compound)
4	--	Individual Compound (Variant, Derivative, or Main Compound)
5	--	Full Record
6	Free	Compound Name, CAS Registry Number, Data Present
7	Long	Individual Compound (Variant, Derivative, or Main Compound)
8	Short	Compound Name, Synonyms, CAS Registry Number, Data Present, Subfile
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.

<b>USER DEFINED FORMATS</b>	Display codes listed in the Search Options tables can be used to customize output.	TYPE S4/NA,DP/1-10
<b>TAG</b>	Output can be displayed with tags identifying each display field.	TYPE S3/5/1-10 TAG
<b>DIRECT RECORD ACCESS</b>	If the accession number of a specific record is known, it can be used to display the record directly.	TYPE 00007993/2 DISPLAY 00007993/NA,RN PRINT 00007993/9

**FOR ONLINE HELP:**

See HELP FIELDS 303 for searchable fields; HELP FORMAT 303 for output formats; HELP LIMIT 303 for limits; HELP RATES 303 for cost information; HELP SORT 303 for sorts.