

# CHEMSEARCH™ CHEMNAME® ONTAP® CHEMSEARCH™ (FILE 231)

## FILE DESCRIPTION

The chemical substance files on DIALOG, CHEMSEARCH™, File 398, and CHEMNAME®, File 301, are non-bibliographic files of chemical substances registered through Chemical Abstracts Service. Each record describes a single chemical entity, and contains the CAS® Registry Numbers, molecular formula, CA Substance Index Name(s), available synonyms, complete ring data, and other chemical substance information. The primary purpose of these files is to support specific substance searching and various forms of substructure searching in the DIALOG chemical files. The CAS® Registry Number can be very effectively used to search for information about specific chemicals in several DIALOG databases (see DIALINDEX® categories RNCHEM, and CASREGNO).

ONTAP® CHEMSEARCH™, File 231, is available for **ON**line **T**raining **A**nd **P**ractice. It contains 52,951 records. The substances in File 231 correspond to many of those covered in the bibliographic records in File 204, ONTAP® CA SEARCH, as well as other ONTAP® files containing CAS Registry Numbers.

## SUBJECT COVERAGE

CHEMSEARCH, File 398, contains all chemical substances registered since 1957, including substances that have been cited in the CAS literature since 1967.

CHEMNAME, File 301, presently includes those chemical substances in the CAS Registry System cited in Chemical Abstracts two or more times from 1967 through the most recent monthly update. Records for substances in CHEMNAME are also contained in CHEMSEARCH.

## SOURCES

Chemical substance data in these files are derived from the CAS Registry Nomenclature Service and the CAS Component and Ring Analysis Service provided by Chemical Abstracts Service. Also included are value added enhancements such as the number of records in File 399 CA SEARCH, chemical name segmentation, the ability to MAP CAS Registry Numbers and chemical names between files, and added fields such as Element Count, Periodic Index Terms, and Number of Components.

## DIALOG FILE DATA

Inclusive Dates: 1967 forward (File 301)  
1957 forward (File 398)  
Selected records (File 231)  
Update Frequency: Closed (File 231)  
Monthly (Files 301,398)  
File Size: 2,992,583 records as of July 2000 (File 301)  
25,180,294 records as of July 2000 (File 398)  
52,951 records (File 231)

## CONTACT

The chemical substance files are produced by Dialog using data provided by Chemical Abstracts Service. Questions concerning search strategies, file content, or data integrity should be directed to DIALOG or CAS.

Chemical Abstracts Service  
Attn: Customer Service  
P.O. Box 3012  
Columbus, OH 43210  
Phone: 614-447-3731  
Toll Free: 800-753-4227  
E-Mail: help@cas.org

Search Strategy and File Content:  
The Dialog Corporation  
The Knowledge Center  
11000 Regency Parkway, Suite 10  
Cary, NC 27511  
Phone: 919-462-8600  
Toll Free: 800-334-2564  
Fax: 919-468-9890  
E-Mail: customer@dialog.com

**Files 398,301  
SAMPLE RECORD**

**CHEMSEARCH™**

**RN=**  
**/EC, EC=, ME=, MF=**  
**AR=, FR=, IR=, NR=, SR=**  
**RN=, RD=**  
**CN=, NA=, /NA**  
**HP=**  
**SB=**  
**NM=**  
**ST=**  
**HP=**  
**SB=**  
**CN=, NA=, /NA**  
**HP=**  
**SB=**  
**HP=**  
**SB=**  
**NM=**  
**HP=**  
**NM=**  
**SY=, /SY, NA=, /NA**  
**UD=**

DIALOG(R) File 398:CHEMSEARCH(TM)  
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CAS REGISTRY NUMBER: 14325-03-2 (COORD-COMPD)  
MOLECULAR FORMULA: C34H30CoN4O4.2H  
RING SYSTEM DATA:  
(01) (nr=08; sr=5,5,5,5,6,6,6,6; ar=C4N.04-C3CoN2.04;  
fr=NC4.04-CoNC3N.04; ir=9832-11-7)  
REPLACED CAS REGISTRY NUMBER(S) : 7097-74-7 13965-24-7  
CA NAME(S) :  
HP=Cobaltate(2-) (9CI)  
SB=(7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-  
2,18-dipropanoato(4-)-N21,N22,N23,N24)-  
NM=dihydrogen  
ST=(SP-4-2)-  
HP=Cobalt (8CI)  
SB=(dihydrogen 3,7,12,17-tetramethyl-8,13-divinyl-2,18-  
porphinedipropionato(2-))-  
OTHER CA NAMES:  
HP=Cobalt (7CI)  
SB=(dihydrogen protoporphyrin IX-ato(2-))-  
HP=21H,23H-Porphine-2,18-dipropanoic acid  
SB=7,12-diethenyl-3,8,13,17-tetramethyl-  
NM=cobalt complex  
HP=21H,23H-Porphine  
NM=cobalt complex  
SYNONYMS: Cobalt protoporphyrin IX; Cobalt(II) protoporphyrin IX;  
Cobalt-heme  
SUBFILE: CHEMNAME 143 LITERATURE REFERENCE(S) IN FILE 399.  
LAST UPDATE: 199301

**RN=**  
**/EC, EC=, ME=, MF=**  
**AF=, MF=**  
**CN=, AC=, NA=, /NA**  
**HP=**  
**NM=**  
**CN=, AC=, NA=, /NA**  
**HP=**  
**NM=**  
**HP=**  
**NM=**  
**HP=**  
**NM=**  
**SY=, NA=, /NA**  
**RC=**  
**UD=**

DIALOG(R) File 398:CHEMSEARCH(TM)  
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CAS REGISTRY NUMBER: 73064-67-2 (ALLOY)  
MOLECULAR FORMULA: Ag.Au.Cu.Si  
ALTERNATE FORMULA: Unknown  
CA NAME(S) :  
HP=Silver alloy(base) (9CI)  
NM=Ag 82,Au 10,Si 4.9,Cu 3.3  
OTHER CA NAMES:  
HP=Gold alloy(nonbase)  
NM=Ag 82,Au 10,Si 4.9,Cu 3.3  
HP=Silicon alloy(nonbase)  
NM=Ag 82,Au 10,Si 4.9,Cu 3.3  
HP=Copper alloy(nonbase)  
NM=Ag 82,Au 10,Si 4.9,Cu 3.3  
SYNONYMS: Copper 5, gold 5, silicon 17, silver 73 (atomic)  
COMPONENT CAS REGISTRY NUMBER(S):  
(7440-21-3 7440-22-4 7440-50-8 7440-57-5)  
  
Component RN      Component Molecular Formula  
=====

1)	7440-21-3	Si
2)	7440-22-4	Ag
3)	7440-50-8	Cu
4)	7440-57-5	Au

SUBFILE: CHEMSIS 10CI 1 LITERATURE REFERENCE(S) IN FILE 399.  
LAST UPDATE: 199203

## SEARCH OPTIONS

## BASIC INDEX

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
— —	— —	All Basic Index Fields <sup>1</sup> Substance Class Descriptor	Word Phrase	S DIHYDROGEN(W)PROTOPORPHYRIN S COORD-COMP S ALLOY
/EC /NA	— NA	Element Count <sup>2</sup> Chemical Names (includes CA Name and Synonyms) <sup>2,3,4</sup>	Word Segment & Word & Phrase	S N4/EC S PORPHINE/NA S DIHYDROGEN(W)PROTOPORPHYRIN/NA S COBALTATE(2-)/NA
/SY	SY	Synonym <sup>2,3,5</sup>	Segment & Word & Phrase	S PROTO(W)PORPHYRIN/SY S COBALT(W)PROTOPORPHYRIN/SY S COBALT PROTOPORPHYRIN IX/SY

<sup>1</sup> All words are indexed, including the standard Dialog stop words.

<sup>2</sup> Searchable in the Basic Index and in the Additional Indexes.

<sup>3</sup> All chemical names are indexed as complete phrases, individual words, and chemically significant segments of words. Words such as PROTOPORPHYRIN may be searched by either segment, e.g., PROTO or PORPHYRIN; for segments that are also complete words, use /FF, e.g., S PORPHYRIN/FF. Locants, i.e., numbers indicating the position of a chemical group within the structure, are searched as words, e.g., S 21. Locant strings, i.e., multiple positions for a recurring group such as 7,12-DIETHENYL, are searched as a single word, e.g., S 7,12 rather than using proximity operators.

<sup>4</sup> CA Name field contains terms and segments from CA Index Names also indexed in HP=, SB=, and NM= fields; CA Name also may be searched using CN=, NA= and /NA.

<sup>5</sup> Synonym, /SY, field contains complete synonyms and segments of synonyms; SY= and NA= fields contain only the complete synonym name.

## ADDITIONAL INDEXES

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
AC= CN= HP=	— CN —	Alloy Component CA Name <sup>2,6</sup> Heading Parent <sup>2,4,7</sup>	Phrase Phrase Segment & Word & Phrase	S AC=AG 82 S CN=COBALTATE(2-),(7,12-DIETHENYL? S HP=(DI(W)PROPAN(W)OIC) S HP=(DIPROPANOIC(W)ACID) S HP=21H,23H-PORPHINE-2,18?
NA= NM=	NA —	Chemical Names (CA Name and Synonyms) <sup>2,4</sup> Name Modification <sup>2,4,7</sup>	Phrase Segment & Word & Phrase	S NA=COBALT-HEME S NM=(DI(W)HYDROGEN) S NM=(COBALT(W)COMPLEX) S NM=COBALT COMPLEX
— SB=	OC —	Other CA Index Names Substituent <sup>2,4</sup>	Segment & Word & Phrase	S SB=(TETRA(W)METHYL) S SB=(DIETHENYL(S)TETRAMETHYL) S SB=7,12-DIETHENYL-3,8,13,17-TETRA?
ST=	—	Stereochemical Descriptor <sup>4</sup>	Word & Phrase	S ST=SP S ST=(SP-4-2)-
SY=	SY	Synonym <sup>2,5</sup>	Phrase	S SY=COBALT-HEME

## MOLECULAR FORMULA DATA

AF= EC= GN= ME= MF=	AF — — — MF	Alternate MF Element Count <sup>2</sup> Group Number Molecular Element Molecular Formula <sup>8</sup>	Phrase Phrase Phrase Phrase Phrase	S AF=UNKNOWN S EC=C0034(S)EC=O0004 S GN=A5 S ME=CHCONO S MF=C34H30CON4O4.2H S MF=C34H30CON4O4 S MF=UNKNOWN
NC= NE= PI=	— — —	Number of Components Number of Elements Periodic Index Term	Phrase Phrase Phrase	S NC=02 S NE=05 S PI=A56 S PI=A56B8
PT=	—	Periodic Transition Row	Phrase	S PT=T1

## RING DATA

— AR=	— —	Ring System Multiplier Analysis of Rings	Word Phrase	S 01(S)AR=C4N.04-C3CON2.04 S AR=C4N.04-C3CON2.04
CR= ER= FR= IR=	— — — —	Component of Rings Elements of Rings Formula of Rings Identity of Rings	Phrase Phrase Phrase Phrase	S CR=CCON S ER=N0004 S FR=NC4.04-CONC3N.04 S IR=9832-11-7 S IR=9832
NR= —	— RS	Number of Rings Ring System Data <sup>9</sup>	Phrase	S NR=08

## ADDITIONAL INDEXES (cont'd)

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
SR=	—	Size of Rings	Phrase	S SR=5,5,5,5,6,6,6,6
TR=	—	Total Number of Rings	Phrase	S TR=08
<b>CAS REGISTRY NUMBER DATA</b>				
ON=	ON	Other Registry Number <sup>13</sup>	Phrase	S ON=7097-74-7
RA=	RA	Alternate Registry Number	Phrase	S RA=10031-75-1
RC=	RC	Component Registry Number <sup>12</sup>	Phrase	S RC=7440-21-3
RD=	RD	Replaced Registry Number	Phrase	S RD=7097-74-7
RF=	RF	Fragment Registry Number	Phrase	S RF=20683-82-3
RG=	RG	Replacing Registry Number	Phrase	S RG=14325-03-2
—	RM	Main Registry Number		
RN=	RN	CAS(R) Registry Number <sup>10,11,13,14</sup>	Phrase	S RN=73064-67-2 S RN=14325-03-2
RP=	RP	Preferred Registry Number	Phrase	S RP=10045-95-1
<b>OTHER DATA</b>				
—	RE	Number of References		
—	SF	Subfile (Collective Index)		
UD=	UD	Update	Phrase	S UD=199301

<sup>6</sup> CA Name is CA Index Names HP=, SB=, and NM= terms separated by commas.

<sup>7</sup> Chemical names are indexed as complete phrases, individual words, and chemically significant segments of words. Use /FW, Full Word, to limit to the unsegmented term. Note, use of /FW is valid only for HP=, SB=, and NM=; for all other fields use /FF to limit to unsegmented chemical terms. Locant strings, such as 7,12 in 7,12-DIETHENYL, are searched as a single word, e.g., SELECT 7,12(W)DIETHENYL.

<sup>8</sup> Includes AF=.

<sup>9</sup> Use the RS display code to display ALL Ring System data.

<sup>10</sup> RN= searches all Registry Numbers except RC= or RF=; RN display Code displays all Registry Numbers except RC or RF.

<sup>11</sup> Use /FF to limit the search to the main CAS Registry Number, e.g., S RN=14325-03-2/FF.

<sup>12</sup> Includes RF=.

<sup>13</sup> Includes RA=, RD=, RG=, and RP=.

<sup>14</sup> MAP RN maps all Registry Numbers in a record except RC (Component Registry) and RF (Fragment Registry) Numbers.

## SPECIAL FEATURES

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

<b>LIMIT</b>	/PLM -- Polymers /STE -- Stereochemical Descriptors	SELECT S4/PLM SELECT S2/STE
<b>SORT</b>	MF, RN, TR	SORT S4/ALL/TR PRINT S2/5/1-24/MF/RN
<b>RANK</b>	All phrase- and numeric-indexed fields in the Additional Indexes can be ranked. Other RANK codes include: RN, SYRN	RANK NA RANK MF S4
<b>MAP</b>	IR, RC, RN, SY, SYRN	MAP SY TEMP S2

## PREDEFINED FORMAT OPTIONS

NO.	DIALOGWEB FORMAT	RECORD CONTENT
1	--	DIALOG Accession Number (not meaningful)
2	--	CAS Registry Number, Other CAS Registry Numbers (except Component or Fragment Registry Numbers), Molecular Formula, Ring System Data, CA Index Name(s) (excluding other CA Names), all Synonyms, Subfile, and Number of References in File 399
3	Medium	CAS Registry Number, Other CAS Registry Numbers (except Component or Fragment Registry Numbers), Molecular Formula, Ring System Data, CA Index Name(s) (excluding other CA Names), all Synonyms, Subfile, and Number of References in File 399
5	--	Full Record
6	--	CAS Registry Number, Molecular Formula, CA Index Name(s), Subfile, and Number of References in CA SEARCH (File 399)
7	Long	CA Index Name(s) (excluding other CA Names) and Ring System Data
8	Short	CA Index Name(s) (excluding other CA Names)
9	Full	Full Record

**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 S3/RN,MF,SY/1-5
<b>TAG</b>	Output can be displayed with tags identifying each display field.	TYPE S2/5/1-6 TAG
<b>DIRECT RECORD ACCESS</b>	Direct Record Access is not applicable in Files 398, 301, and 231.	

**FOR ONLINE HELP:**

See HELP FIELDS 398 for searchable fields; HELP FORMAT 398 for output formats; HELP LIMIT 398 for limits; HELP RATES 398 for cost information; HELP SORT 398 for sorts.