

# CHEMSEARCH™

## ONTAP® CHEMSEARCH™ (FILE 231)

### FILE DESCRIPTION

The chemical substance file on DIALOG, CHEMSEARCH™, File 398, is a non-bibliographic file of chemical substances registered through Chemical Abstracts Service.

Each record describes a single chemical entity, and contains the CAS® Registry Number(s), molecular formula, CA Substance Index Name(s), available synonyms, complete ring data, and other chemical substance information. 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.

The primary purpose of this file 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 by the CAS Registry System since 1957, including substances that have been cited in Chemical Abstracts since 1967.

### SOURCES

Chemical substance data in this file is derived from the CAS Registry Nomenclature Service and the CAS Component and Ring Analysis Service (CARAS) provided by Chemical Abstracts Service.

### TIPS

#### BEGIN 398

to search chemical substances and their CAS Registry Numbers.

#### USE MAP RN T

to create a temporary SearchSave of CAS® Registry Numbers for locating the source records in file 399, CASearch.

MAP RN TEMP S3

#### USE MAP SY T

to create a temporary SearchSave of substance synonyms for searching in other files

MAP SY TEMP S3

#### USE RANK SB

to review substituents on a particular Heading Parent  
SELECT HP=COBALTATE; RANK SB

### DIALOG FILE DATA

Inclusive Dates: 1957 forward

Update Frequency: Monthly

File Size: over 100 million records as of March 2009

### 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.

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## SAMPLE SUBSTANCE RECORD

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-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24)-  
NM=dihydrogen  
ST=(SP-4-2)-  
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 (8CI)  
SB=(dihydrogen 3,7,12,17-tetramethyl-8,13-divinyl-2,18-porphinedipropionato(2-))-  
HP=Cobalt (7CI)  
SB=(dihydrogen protoporphyrin IX-ato(2-))-  
HP=Cobaltate(2-)  
SB=(7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24)-  
NM=hydrogen (1:2)  
ST=(SP-4-2)-  
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=cobaltate(2-) deriv.  
SYNONYMS: Cobalt protoporphyrin IX; Cobalt(II) protoporphyrin IX; Cobalt-heme; NSC 267101  
FRAGMENT CAS REGISTRY NUMBER(S):  
(744135-48-6)  
LITERATURE REFERENCE(S) IN CA SEARCH (file 399) = 143  
LAST UPDATE: 200712

## SAMPLE POLYMER RECORD

DIALOG(R)File 398:CHEMSEARCH(TM)  
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CAS REGISTRY NUMBER: 127383-17-9 ( POLYMER )  
MOLECULAR FORMULA: (C6H9NO.C3H4O2)x  
RING SYSTEM DATA:  
(01) (nr=01; sr=5; ar=C4N.01; fr=NC4.01; ir=16-136-1)  
CA NAME(S):  
HP=2-Propenoic acid (9CI)  
NM=polymer with 1-ethenyl-2-pyrrolidinone  
ST=graft  
OTHER CA NAMES:  
HP=2-Pyrrolidinone  
SB=1-ethenyl-  
NM=polymer with 2-propenoic acid  
ST=graft  
SYNONYMS: Acrylic acid-N-vinylpyrrolidone graft copolymer  
COMPONENT CAS REGISTRY NUMBER(S):  
(79-10-7 88-12-0)

Component RN	Component Molecular Formula
1)	79-10-7 C3H4O2
2)	88-12-0 C6H9NO

## SAMPLE POLYMER RECORD (cont'd)

RE= LITERATURE REFERENCE(S) IN CA SEARCH (file 399) = 5  
 UD= LAST UPDATE: 199612

## SAMPLE GENE SEQUENCE RECORD

DIALOG(R)File 398:CHEMSEARCH(TM)  
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RN= CAS REGISTRY NUMBER: 172643-85-5 ( MANL-REGSTD )  
 MF= MOLECULAR FORMULA: Unknown  
 CA NAME(S):  
 HP=DNA (9CI)  
 SB=d(A-G-G-A-C-A-C-A-T-T-G-T-G-C-C)  
 NM=double-stranded complementary  
 HP=Deoxyribonucleic acid  
 SB=d(A-G-G-A-C-A-C-A-T-T-G-T-G-C-C)  
 NM=double-stranded complementary  
 OTHER CA NAMES:  
 HP=DNA  
 SB=d(G-G-C-A-C-A-A-T-G-T-G-T-C-C-T)  
 NM=double-stranded complementary  
 SY=,/SY,NA=,/NA  
 SYNONYMS: Deoxyribonucleic acid (human growth hormone gene hormone-responsive element-containing fragment); Deoxyribonucleic acid (human somatotropin gene hormone-responsive element-containing fragment)  
 RE= LITERATURE REFERENCE(S) IN CA SEARCH (file 399) = 1  
 UD= LAST UPDATE: 200801

## SEARCH OPTIONS

## BASIC INDEX

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
—	—	All Basic Index Fields <sup>1</sup>	Word	S DIHYDROGEN(W)PROTOPORPHYRIN
—	—	Substance Class Descriptor	Phrase	S COORD-COMP S ALLOY
/EC	—	Element Count <sup>2</sup>	Word	S N4/EC
/NA	NA	Chemical Names (includes CA Name and Synonyms) <sup>2,3,4</sup>	Segment & Word & Phrase	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=	—	Alloy Component	Phrase	S AC=AG 82
CN=	CN	CA Name <sup>2,6</sup>	Phrase	S CN=COBALTATE(2-),(7,12-DIETHENYL)?
HP=	—	Heading Parent <sup>2,4,7</sup>	Segment & Word & Phrase	S HP=(DI(W)PROPAN(W)OIC) S HP=(DIPROPANOIC(W)ACID) S HP=21H,23H-PORPHINE-2,18?
NA=	NA	Chemical Names (CA Name and Synonyms) <sup>2,4</sup>	Phrase	S NA=COBALT-HEME
NM=	—	Name Modification <sup>2,4,7</sup>	Segment & Word & Phrase	S NM=(DI(W)HYDROGEN) S NM=(COBALT(W)COMPLEX) S NM=COBALT COMPLEX
—	OC	Other CA Index Names		

## ADDITIONAL INDEXES (cont'd)

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
SB=	—	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? S ST=SP S ST=(SP-4-2)- S SY=COBALT-HEME
ST=	—	Stereochemical Descriptor <sup>4</sup>	Word & Phrase	
SY=	SY	Synonym <sup>2,5</sup>	Phrase	
<b>MOLECULAR FORMULA DATA</b>				
AF=	AF	Alternate MF	Phrase	S AF=UNKNOWN
EC=	—	Element Count <sup>2</sup>	Phrase	S EC=C0034(S)EC=O0004
GN=	—	Group Number	Phrase	S GN=A5
ME=	—	Molecular Element	Phrase	S ME=CHCONO
MF=	MF	Molecular Formula <sup>8</sup>	Phrase	S MF=C34H30CON4O4.2H S MF=C34H30CON4O4 S MF=UNKNOWN
NC=	—	Number of Components	Phrase	S NC=02
NE=	—	Number of Elements	Phrase	S NE=05
PI=	—	Periodic Index Term	Phrase	S PI=A56 S PI=A56B8
PT=	—	Periodic Transition Row	Phrase	S PT=T1
<b>RING DATA</b>				
—	—	Ring System Multiplier	Word	S 01(S)AR=C4N.04-C3CON2.04
AR=	—	Analysis of Rings	Phrase	S AR=C4N.04-C3CON2.04
CR=	—	Component of Rings	Phrase	S CR=CCON
ER=	—	Elements of Rings	Phrase	S ER=N0004
FR=	—	Formula of Rings	Phrase	S FR=NC4.04-CONC3N.04
IR=	—	Identity of Rings	Phrase	S IR=9832-11-7 S IR=9832
NR=	—	Number of Rings	Phrase	S NR=08
—	RS	Ring System Data <sup>9</sup>		
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=	RE	Number of References <sup>15</sup>	Numeric	S RE=5
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.

<sup>15</sup> RE= is not available in In ONTAP Chemsearch (File 231).

**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 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.