### **DCR** (Derwent Chemistry Resource)



#### Subject Coverage

Organic and inorganic chemical compounds

 Basic compounds, salts and mixtures as well as oligomers with less than 9 repeating groups, enzymes, proteins, chemically modified polysaccharides and standard polymers

File Type

Structure

**Features** 

Alerts (SDIs)

Monthly, weekly, or with each update (2 updates per week)

(every update is the default).

In addition, SMARTracker, an automatic crossfile current awareness

search, (SDI XFILE) using a DCR search profile in

WPINDEX, WPIX and WPIDS may be run every update, weekly or

biweekly (every update is the default).

CAS Registry Number® Identifiers

<u>SLART</u>

 $\overline{\checkmark}$ 

 $\square$ 

Keep & Share

Structures

Record Content

- Chemical compounds from Derwent World Patents Index (DWPI) documents
- DCR numbers unique identifiers for specific chemical compounds and link to corresponding DWPI database records
- Systematic chemical names, commonly used chemical names and synonym names
- Molecular formulas
- Structure diagrams
- Specific structure identifiers
- Substance descriptors
- Controlled terms

File Size

More than 6.2 million specific chemical compounds (04/2025)

Coverage

- 1999-present
- Partial coverage 1981-present: Commonly used and significant compounds
- Chemical structure diagrams 1992-present

**Updates** 

Updated twice a week with about 3,900 new chemical compounds

Language

English

Database

Clarivate

**Producer** Friars House, 160 Blackfriars Rd.

London SE1 8EZ

United Kingdom

Copyright Holder: Clarivate

Sources

Claims and examples of patents indexed in the Derwent World Patents Index (DWPI)

and classified in Chemical Patents Index (CPI) Sections B (Pharmaceuticals).

C (Agrochemicals) and/or E (General Chemicals)

**User Aids** 

Online Helps (HELP DIRECTORY lists all help messages available)

STNGUIDĖ

Cluster

STRUCTURE

STN Database Cluster information

Related Databases WPINDEX, WPIDS, WPIX

## **Search and Display Fields**

Fields that allow left truncation are indicated by an asterisk (\*).

| Search Field Name  | Search<br>Code                          | Search Examples  | Display<br>Codes                                 |
|--|---|--|--|
| Basic Index * (contains single terms from CN, CMT, MF and SCT)   | None<br>(or /BI)                        | S ?PHENYLETHER?<br>S UBIQUINONE/CMT<br>S C19H19FN2O2S<br>S ACETYLCHOLINE-RECEPTOR                          | CMT, CN.P,<br>CN.S, MF,<br>SCT.DA,<br>SCT.MA, SY |
| Accession Number (DCR Number) Chemical Name (CN.P, CN.S, SY) Chemical Name Segment * (from CN)           | /AN<br>/CN<br>/CNS                      | S DCR-5303196/AN<br>S MANDELIC ACID/CN<br>S DISULFONYL DIAZIDE/CNS   | AN<br>CN.P,CN.S,SY<br>CN.P,CN.S,SY               |
| Chemical Name, Preferred<br>Chemical Name, Synonym<br>Chemical Name, Systematic<br>Comment               | /CN.P<br>/SY<br>/CN.S<br>/CMT           | S D-GLUCOSE-6-PHOSPHATE/CN.P<br>S FALUBIN/SY<br>S DECANE-1,10-DISULFONYL DIAZIDE/CN.S<br>S FIBROBLAST#/CMT | CN.P<br>SY<br>CN.S<br>CMT                        |
| Component Molecular Formula  | /CMF (or<br>/FRAGMF)                    | S C H3 F6 P/CMF  | CMF  |
| Component Molecular Formula, Count   | /CMF.CNT                                | S 6/CMF.CNT  | CMF  |
| Controlled Term, Substance<br>(SCT.DA, SCT.MA)   | /SCT (/CT)                              | S MAO-INHIBITOR/SCT  | SCT.DA,<br>SCT.MA                                |
| Controlled Term, Substance, Drug Activity  | /SCT.DA (or /CT.DA)                     | S MAP-KINASE-INH?/SCT.DA   | SCT.DA   |
| Controlled Term, Substance, Mechanism of Action  | /SCT.MA (or /CT.MA)                     | S ADRENALINE/SCT.MA  | SCT.MA   |
| Derwent Compound Number,<br>Substance (2)  | /SDCN                                   | S R20123/SDCN  | SDCN   |
| Derwent Drug Registry Name<br>Derwent Registry Number,<br>Substance (2)                                  | /DDRN<br>/SDRN                          | S 2-184/DDRN<br>S 1029/SDRN  | DDRN<br>SDRN                                     |
| Element Count (1) Element Count Substance (1) Element Symbol Element Symbol, Count (1)                   | /ELC<br>/ELC.SUB<br>/ELS<br>/ELS.CNT    | S (S AND O AND C AND H)/ELS AND 4/ELC S (S AND C AND H)/ELS AND 4/ELC.SUB S FE/ELS S O/ELS(S)7/ELS.CNT     | MF<br>MF<br>MF<br>MF                             |
| Entry Date, Chemistry Resource (1)   | /ED (or<br>/EDCR)                       | S 20210323/ED  | ED   |
| Field Availability<br>InChIKey   | /FA<br>/INKY (or<br>/INCHI)             | S DDRN/FA<br>S FXEBTZMNJRTVTM/INKY   | Not displayed INCHI, INKY                        |
| Molecular Formula<br>Molecular Weight (1)<br>Number of Components (1)<br>Number of Components, Total (1) | /MF<br>/MW<br>/NC<br>/NC.TOT            | S H CL2 N/MF<br>S 17-21/MW<br>S 9-11/NC<br>S 4/NC.TOT AND L11  | MF<br>MW<br>SMF<br>SMF                           |
| Periodic Group Ring Index Number, Substance (2) Standardized Molecular Formula                           | /PG<br>/SRIN<br>/SMF                    | S A2/PG<br>S 11895/SRIN<br>S "B *1; SI *1; TOTAL *2; TYPE *2"/SMF  | Not displayed<br>SRIN<br>SMF                     |
| Structured DCR Number Substance Descriptor Substructure Terms Update Date, DCR (1,3)                     | /DCSE<br>/SD (or /CC)<br>/SS<br>/UP (or | S 70-0-0/DCSE<br>S HALOCARBONS/SD<br>S PHOSPHONIC-ACID/SS<br>S JAN 2000/UP                                 | DCSE<br>SD<br>SS<br>UP                           |
| Update Date, DWPI Cross Reference (1,4)  | /UPCR)<br>/UPWX                         | S 19990719/UPWX  | UPWX   |

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

<sup>(2)</sup> Cross reference to indexing in bibliographic records. Select data from SDCN or SDRN or SRIN and search in /DCN resp. /DRN, resp. /RIN to retrieve bibliographic records.

<sup>(3)</sup> UPCR is created when existing records are updated or when new compounds enter the Chemistry Resource Segment.

<sup>(4)</sup> UPWX is created when DCR compounds are cited in bibliographic records. UPWX may be used in automatic current awareness searches (SDIs) in the Chemistry Resource Segment.

## **Structure Searching**

| Terms   | Search Examples    |
|---|--------------------|
| L-numbers of structures built using the STRUCTURE editor in STNext  | SEARCH L1 FAM      |
| L-numbers of structures built using the STRUCTURE command (Boolean logic allowed between L-numbers)   | SEA L1 AND L2 SSS  |
| L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)   | S L3 OR L4 SSS     |
| L-numbers of structures built using the STRUCTURE command combined with L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers) | S L1 AND L2 NOT L3 |

## **Types of Structure Searching**

| Туре                      | Definition  | Search<br>Code | Search Examples                                    |
|---------------------------|---|----------------|--|
| Substructure<br>(default) | Search for substances which match the query. Substitution is allowed at all open positions. Additional components may be retrieved.   | SSS            | SEARCH L1 SSS<br>S L2 OR L3 SSS<br>S L7 SSS        |
| Closed<br>Substructure    | Search for substances which match the query exactly. Substitution is allowed at positions by assigning non-hydrogen attachments. Right click on a node or group of nodes and use the Non-Hydrogen Count tab in the STNext structure drawing tool. Additional components may be retrieved. | CSS            | SEARCH L1 CSS<br>S L2 NOT L3 CSS<br>S L4 OR L5 CSS |
| Exact                     | Search for substances which match the query exactly   | EXA            | S L5 EXA FUL                                       |
| Family                    | Search for substances which match the query exactly. Additional components may be retrieved.  | FAM            | S L6 FAM   |

# **Scopes of Structure Searching**

| Scope               | Definition   | Search<br>Code | Search Examples     |
|---------------------|--|----------------|---------------------|
| Sample<br>(default) | Search a fixed 10% of the file (a maximum of 50 records displayed) | SAM            | S L6 SSS SAM        |
| Full                | Search 100% of the file  | FUL            | S L5 OR L8 SSS      |
| Subset Sample       | Search a fixed sample of an answer set created by a search in DCR  | SUB SAM        | S L7 SSS SUB=L5 SAM |
| Subset Full         | Search 100% of an answer set created by a search in DCR            | SUB FUL        | S L7 SSS SUB=L5 FUL |

#### **DISPLAY and PRINT Formats**

Any combination of formats may be used to display or print answers. Multiple codes must be separated by spaces or commas, e.g., D L1 1-5 TI AU. The fields are displayed or printed in the order requested.

Hit term highlighting is available for all fields. Highlighting must be ON during SEARCH to use the HIT, KWIC, and OCC formats.

| Format       | Content  | Examples    |
|--------------|--|-------------|
| AN           | Accession Number (DCR Number)  | D AN        |
| CMT          | Comment  | D CMT       |
| CN (1)       | Chemical Name (includes CN.P,CN.S and SY)  | D CN        |
| CN.P (1)     | Chemical Name, Preferred   | D CN.P      |
| CN.S (1)     | Chemical Name, Systematic  | D CN.S 1-5  |
| DCSE ,       | Structured DCR Number  | D DCSE      |
| DDRN         | Derwent Drug Registry Name   | D DDRN 1-2  |
| ED (EDCR)    | Entry Date, Chemistry Resource   | D ED        |
| INCH         | InChI Code   | D INCH      |
| INKY (INCHI) | InChlKey   | D INKY      |
| MF ,         | Molecular Formula  | D MF        |
| MW           | Molecular Weight   | D MW        |
| SCT (CT)     | Controlled Term, Substance (includes SCT.DA and SCT.MA)  | D SCT       |
| SD (CC)      | Substance Descriptor   | D SD        |
| SDĈN         | Derwent Compound Number, Substance   | D SDCN      |
| SDRN         | Derwent Registry Number, Substance   | D SDRN      |
| SMF          | Standardized Molecular Formula   | D SMF       |
| SRIN         | Ring Index Number, Substance   | D SRIN 1-10 |
| SS           | Substructure Terms   | D SS        |
| STR          | Chemical Structure Display   | D STR       |
| SY (1)       | Chemical Name, Synonym   | D SY        |
| UP (ÚPCR)    | Update Date, DCR   | D UP        |
| UPWX ´       | Update Date, DWPI Cross Reference  | D UPWX      |
|              |  |             |
| ALL (FULL)   | AN, DCSE, CN.P, CN.S, SY, STR, CMT, MF, SMF, INCH, INKY, MW,   | D ALL       |
|              | SRIN, SDCN, SDRN, SD, ED, UP, UPWX   | 5           |
| IALL         | ALL, indented with text labels   | D IALL      |
| MAX          | AN, DCSE, CN.P, CN.S, SY, STR, CMT, MF, SMF, INCH, INKY, MW,   | D MAX       |
|              | SRIN, SDCN, SDRN, DDRN, SD, SCT.DA, SCT.MA, SS, ED, UP,  |             |
| INAAN        | UPWX   | DIMAY       |
| IMAX         | MAX, indented with text labels   | D IMAX      |
| STD (IDE)    | AN, DCSE, CN.P, CN.S, SY, STR, CMT, MF, INCH, INKY, ED, UP, UPWX   | D STD 1-4   |
| IOTO         | (STD is the default)   | D IOTO      |
| ISTD         | STD, indented with text labels   | D ISTD      |
| SCAN (2)     | CN.S, MF, STR (random display without answer number)   | D SCAN      |
| SAMPLE (SAM) | CN.S, MF, STR  | D SAM       |
| HIT          | Hit term(s) and field(s)   | D HIT       |
| KWIC         | Up to 50 words before and after hit term(s) (KeyWord-In-Context)   | D KWIC      |
| OCC          | Number of occurrences of hit term(s) and field(s) in which they occur  | D OCC       |
|              | Trained of occasionous of the configuration mode of the configuration of | 2 300       |

<sup>(1)</sup> All Chemical Names, .Preferred, Systematic and Synonym, are displayed with the CN display code. (2) SCAN must be specified on the command line, i.e., D SCAN or DISPLAY 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/<br>SELECT (1) | SORT |
|------------------------------------|--------------|------------------------|------|
| Accession Number (DCR number)      | AN           | Υ                      | Υ    |
| Chemical Name                      | CN           | Y (2)                  | Ν    |
| Chemical Name, Preferred           | CN.P         | Υ                      | Ν    |
| Chemical Name, Synonym             | SY           | Υ                      | Ν    |
| Chemical Name, Systematic          | CN.S         | Υ                      | Ν    |
| Comment                            | CMT          | Υ                      | Ν    |
| Controlled Term, Substance         | SCT          | Y (3)                  | Ν    |
| Derwent Compound Number, Substance | SDCN         | Υ                      | Υ    |
| Derwent Drug Registry Name         | DDRN         | Υ                      | Ν    |
| Derwent Registry Number, Substance | SDRN         | Υ                      | Υ    |
| Entry Date, Chemistry Resource     | EDCR (ED)    | Υ                      | Υ    |
| InChlKey                           | INKY (INCHI) | Υ                      | Ν    |
| Molecular Weight                   | MW           | Υ                      | Υ    |
| Number of Components               | NC           | N                      | Υ    |
| Ring Index Number, Substance       | SRIN         | Υ                      | N    |
| Standardized Molecular Formula     | SMF          | Υ                      | Ν    |
| Structured DCR Number              | DCSE         | Υ                      | Υ    |
| Substance Descriptor               | SD           | Υ                      | Ν    |
| Update Date, DCR                   | UPCR (UP)    | Υ                      | Υ    |
| Update Date, DWPI Cross Reference  | UPWX` ´      | Υ                      | Υ    |

<sup>(1)</sup> 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.

<sup>(2)</sup> Selects or analyzes CN.S, CN.P and SY with /CN appended to the terms created by SELECT.

<sup>(3)</sup> Selects or analyzes SCT.DA and SCT.MA with /SCT appended to the terms created by SELECT.

### Sample Records

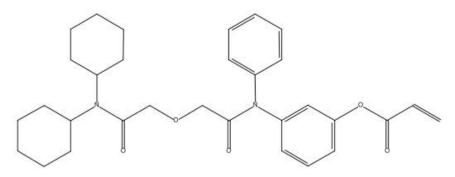
#### **DISPLAY ALL**

L8 ANSWER 1 OF 1 DCR COPYRIGHT 2025 CLARIVATE on STN.

AN DCR-1000003 DCF DCSE 1000003-0-0-0

CN.S Acrylic acid 3-({[(dicyclohexylcarbamoyl)-methoxy]-acetyl}-phenyl-amino)-phenyl

ester



MF C31 H38 N2 O5

SMF TYPE \*1; C31 H38 N2 O5 \*1; TOTAL \*1

INCH InChI=1S/C31H38N2O5/c1-2-31(36)38-28-20-12-19-27(21-28)33(26-17-10-5-11-

25/h2,5,10-12,17-21,24-25H,1,3-4,6-9,13-16,22-23H2

INKY BUUIFPGRUSICSX-UHFFFAOYSA-N

MW 518.6589 SDCN RAG9YE

SD UNSATURATED FATTY ACIDS ED Entered STN: 24 Jan 2005

Last updated on STN: 24 Jan 2005 Update DWPI Cross Ref.: 24 Jan 2005

#### **DISPLAY IMAX**

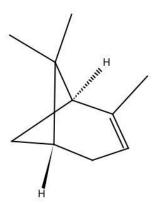
L11 ANSWER 1 OF 1 DCR COPYRIGHT 2024 CLARIVATE on STN.

ACCESSION NUMBER: DCR-4436 DCR STRUCTURED DCR NO.: 4436-0-0-0 PREF. CHEMICAL NAME: ALPHA-PINENE

SYSTEMATIC NAME: 2,6,6-Trimethyl-bicyclo[3.1.1]hept-2-ene

SYNONYMS: ALPHA PINEN; ALPHA-PINEN; ALPHA-PINENE; PINENE,

ALPHA-; PINENE, ALPHA-; PINENE-ALPHASTR



COMMENT: Unspecified stereochemistry

MOLECULAR FORMULA: C10 H16

STANDARD MOL. FORMULA: C10 H16 \*1; TOTAL \*1; TYPE \*1

INCHI CODE: InChI=1S/C10H16/c1-7-4-5-8-6-9(7)10(8,2)3/h4,8-9H,5-

6H2,1-3H3/t8-,9-/m1/s1

INCHI KEY: GRWFGVWFFZKLTI-RKDXNWHRSA-N

MOLECULAR WEIGHT: 136.2364

RING INDEX NUMBER: 00832 DERWENT COMPOUND NO.: R00477 DERWENT REGISTRY NO.: 0477 DERWENT DRUG REG. NAME: PINENEALP SUBSTANCE DESCRIPTOR: TERPENES

SCT, DRUG ACTIVITY: ACETYLCHOLINESTERASE-INHIBITORS; ANALGESICS;

ANTICHOLINESTERASES; CHOLINESTERASE-INHIBITORS;

**FUNGICIDES** 

SCT, MECHANISM OF ACTION: ACETYLCHOLINESTERASE-INHIBITOR; ANTICHOLINESTERASE;

CHOLINESTERASE-INHIBITOR

SUBSTRUCTURE TERM: BRIDGE-STRUCT.; CYCLOBUTANE; CYCLOHEXANE; OLEFIN;

TERPENE

ENTRY DATE: Entered STN: 3 May 1999

Last updated on STN: 12 Aug 2022 Update DWPI Cross Ref.: 25 Mar 2025

In North America

CAS Customer Center: P.O. Box 3012 Columbus, Ohio 43210-0012

U.S.A.

Phone: 800-753-4227 (North America) 614-447-3731 (worldwide)

help@cas.org E-mail: Internet: www.cas.org

In Europe

CAS Customer Center EMEA

FIZ Karlsruhe - Leibniz-Institute for Information Infrastructure
Hermann-von-Helmholtz-Platz 1

76344 Eggenstein-Leopoldshafen

Germany

Phone: +49-721-9588 3155 E-mail: EMEAhelp@cas.org Internet: www.fiz-karlsruhe.de

In Japan

JAICI (Japan Association for International Chemical Information)

Nakai Building 6-25-4 Honkomagome, Bunkyo-ku

Tokyo 113-0021 Japan

+81-3-5978-3601 (Technical Service) +81-3-5978-3621 (Customer Service) Phone: E-mail:

support@jaici.or.jp (Technical Service) customer@jaici.or.jp (Customer Service)

Internet: www.jaici.or.jp