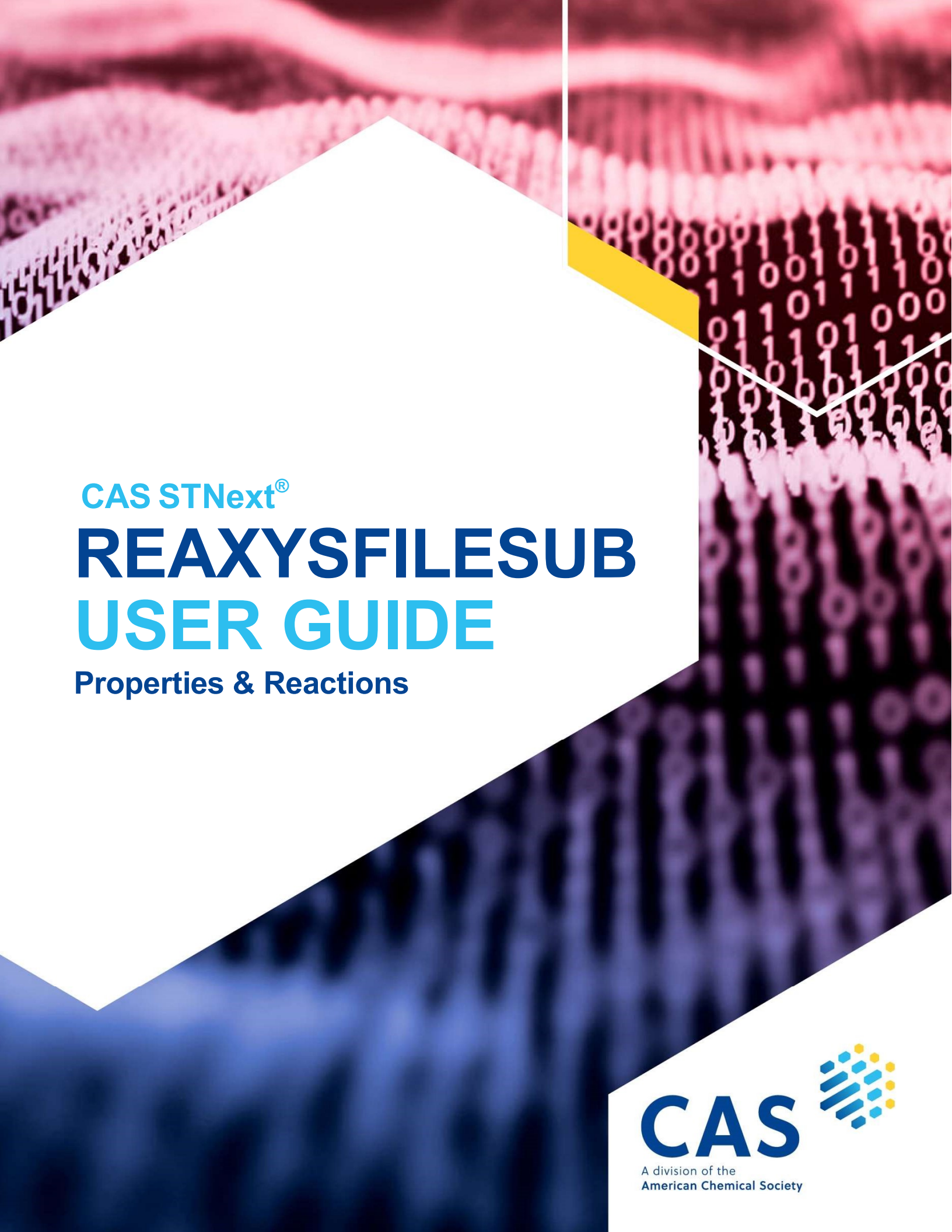


CAS STNext®

REAXYSFILESUB USER GUIDE

Properties & Reactions

CAS
A division of the
American Chemical Society

Searching Properties and Reactions in REAXYSFILESUB on CAS STNext

Content

Summary

Three easy steps to retrieve property and reaction information:

- Combine results of a structure search or of a search with IDE fields with required properties and/or reactions using FA.P and FA.RX, respectively
- DISPLAY QRD (default)
- Possibly check with DISPLAY ALL/IALL for further available properties or reactions

Before you start - some important facts

REAXYSFILESUB contains a large number of properties and reactions - for many substances the number of entries overall or for individual properties is high. The following are tips for better handling of displays.

There are two recommended display formats:

- QRD (query related display)
- ALL, IALL (identification of substance plus field availability list)

DISPLAY FULL is not ordinarily recommended.

Options exist for displaying all of the properties in each of five categories.

Note that there is no crossover option - properties and reactions cannot be transferred from REAXYSFILESUB to REAXYSFILEBIB.

1. **Strongly recommended for displaying properties and reactions: Query Related Display - QRD (default display format)**

   The QRD format should be used to see information pertinent to the conducted search without having to remember the field codes or display formats that might be associated with the data needed.

2. **For an overview of available information – Use DISPLAY ALL or IALL (field names with labels)**
   Display includes Identification of substance plus field availability list, see first entry in list below:
   - Field Code (e.g., DEN) for search and display
   - Property name (e.g., Density of the Liquid)
   - Number of entries (1)
   - Category (e.g., PHYS)
   - Availability of reactions lists number of reaction documents (there is no distinction between product and reactant).

```
ACCESSION NUMBER:       38153   REAXYSFILESU ACCESSION NUMBER:       38153
REAXYSFILESU
REGISTRY NUMBER:        29820-79-9
CHEMICAL NAME:          1,4-Bis03C; 3B2; -(2-quinolyl)vinyl03E; benzene;
                        1,4-di-03C; 3B2; -(2-quinolyl)vinyl03E; benzene;
                        2,2'-(1,4-phenylenedivinylene)bisquinoline;
                        1,4-bis-((i)trans-2-[2]quinolyl-vinyl)-benzene
SUBSTANCE DESCRIPTOR:   heterocyclic
COMP. MOL. FORMULA:     C28 H20 N2
LIN. STRUCTURE FORMULA: C28H20N2
INCHI KEY:              DJDHBLKJOAHWQU-HBKJEHTGSA-N
ALTERNATE INCHI KEY:    DJDHBLKJOAHWQU-HBKJEHTGBR
MOLECULAR WEIGHT:       384.48
MARKUSH REF. COUNT:     1
REFERENCE COUNT:        12
ENTRY DATE:             Entered STN: 14 Jul 2020
                        Last updated on STN: 1 Feb 2024

                           >>structure image<<

PROPERTIES:             DEN Density of the Liquid (1) (PHYS)
                        MP Melting Point (3) (PHYS)
                        FLUS Fluorescence spectroscopy (14) (SPEC)
                        LUM Luminescence spectroscopy (1) (SPEC)
                        NMR NMR spectroscopy (4) (SPEC)
                        UVS UV/VIS spectroscopy (18) (SPEC)
                        CRYPH Crystal Phase (1) (STATE)
                        CPD Crystal Property Description (5) (STATE)
                        CSG Crystal Space Group (1) (STATE)
                        CSYS Crystal System (1) (STATE)
                        POT Electrochemical Characteristics (2) (FURTHER)
                        FINFO2 Further Information (8) (FURTHER)
                        IDA Interatomic Distances and Angles (1) (FURTHER)
                        PSD Patent Specific Data (3) (FURTHER)
                        LB Substance Label (3) (FURTHER)
REACTIONS:              RX.ID; RX.PAN; RX.RAN (2)
```

3. **Not ordinarily recommended: DISPLAY FULL (display of all available information)**
   (Note that IFULL display format is not currently available)
   IMPORTANT: D FULL displays can be very lengthy (> 10,000 entries overall) and might cause a system error. Please check D ALL for the number of property/reaction data entries before using this display format.

```
AN     1205685   REAXYSFILESU
CN     13,13'-dihydroxy-[14,14']biibogaminyl-18,18'-dicarboxylic acid dimethyl
       ester
SD     heterocyclic
MF     C42 H52 N4 O6
CMF    C42 H52 N4 O6
LSF    C42H52N4O6
INCHI  KHWRBQXEKRQJSZ-FPDPKCOBSA-N
AINCHI KHWRBQXEKRQJSZ-FPDPKCOBBI
MW     708.898
MARKREF.CNT 0
REC    1
ED     Entered STN: 13 Jul 2020
       Last updated on STN: 19 Jan 2024

>>structure image<<


PROPERTIES
       ORP Optical Rotatory Power (1) (PHYS)
       IR IR spectroscopy (1) (SPEC)
       MS Mass Spectrometry (1) (SPEC)
       NMR NMR spectroscopy (2) (SPEC)
       UVS UV/VIS spectroscopy (1) (SPEC)
       LB Substance Label (1) (FURTHER)


Optical Rotatory Power (1)
 Value      | Type       | Wavelength | Ref(s)
 (ORP)      | (.TYP)     | (.W)       | (REF)
 (deg)      |            | (nm)       |
============+============+============+============
 -43        | [alpha]    | 589        | 1

1. AN 3007390: Journal: Damak et al., Tetrahedron Lett. (1974), 2141p.

IR spectroscopy (1)
 Keyword    | Ref(s)
 (.KW)      | (REF)
============+============
 IR         | 1

1. AN 3007390: Journal: Damak et al., Tetrahedron Lett. (1974), 2141p.

Mass Spectrometry (1)
 Ref(s)
 (REF)
============
 1
```

```
1. AN 3007390: Journal: Damak et al., Tetrahedron Lett. (1974), 2141p.

NMR spectroscopy (2)
 Keyword     | Comment     | Ref(s)
 (.KW)       | (.CMT)      | (REF)
=============+=============+============
 NMR         | 13C-NMR     | 1
 NMR         |             | 1


1. AN 3007390: Journal: Damak et al., Tetrahedron Lett. (1974), 2141p.

UV/VIS spectroscopy (1)
 Keyword     | Ref(s)
 (.KW)       | (REF)
=============+============
 UV/VIS      | 1


1. AN 3007390: Journal: Damak et al., Tetrahedron Lett. (1974), 2141p.

Substance Label (1)
 Label       | Ref(s)
 (.LB)       | (REF)
=============+============
 1           | 1

1. AN 3007390: Journal: Damak et al., Tetrahedron Lett. (1974), 2141p.

Reaction:
       Reaction ID:                    6393128
       Product AN (.PAN):              1205685
       Product (.PRO):                 13,13'-dihydroxy-[14,14']biibogaminyl-
                                       18,18'-dicarboxylic acid dimethyl ester
       Reference Count:                1

Reaction Details:
       Reaction RID:                   6393128.1
       Reaction Classification (.CL): Preparation (half reaction)
       Reference(s):                   3007390: Journal: Damak et al.,
                                       Tetrahedron Lett. (1974), 2141p.
```

4. **Display of all properties summarised in a category**
   All of the properties in a particular category of properties can be displayed by using the display formats below:

Kind of Property	Description	Example
PHYS	All physical properties	D PHYS
STATE	All state of aggregation properties	D STATE
FURTHER	All further properties	D FURTHER
MULTI	All multicomponent properties	D MULTI
SPEC	All spectroscopy properties	D SPEC

Overview of Properties

Content

The selection of relevant data for the database is very diverse. Single and multicomponent systems are considered. The 110 properties available can be classified into five categories:

- Physical properties (e.g., melting point, boiling point)
- State of aggregation (e.g., crystal data)
- Spectroscopy (e.g., NMR, IR)
- Multicomponent Systems (e.g., electrical data, liquid/liquid systems)
- Further properties (e.g., isolation from natural product, chemical derivative)

Please note: FURTHER INFORMATION FINFO, FINFO1-3 are a collection pool for rarely examined properties, not to be confused with category FURTHER PROPERTIES. The numbers in the names are for technical reasons.

Handling property data with helpful search fields

Summary

Search for a specific property with

/FA.P Field Availability for properties (see example 1 and 3)

Search for keyword(s) with

/KW Keywords of all property fields (see example 2)

Several search and display fields were generated to enhance user-friendliness in dealing with property information:

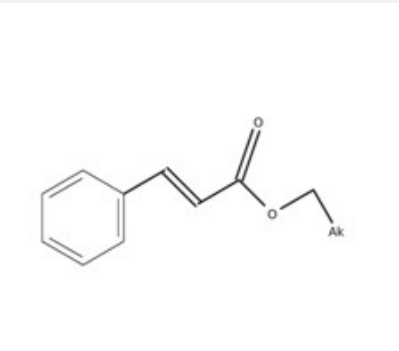
1. **Field Availability for Properties (/FA.P)**

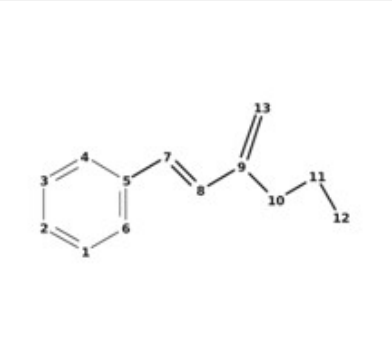
   Indicated in /FA.P are all search/display fields with names and codes. The FA list shows all properties and corresponding occurrences for the given compound. The use of /FA.P is advisable if only records with information for a special property are desired from a hit record set.

   Example 1:

   Search for cinnamic acid alkyl esters with information on melting points (closed substructure search).

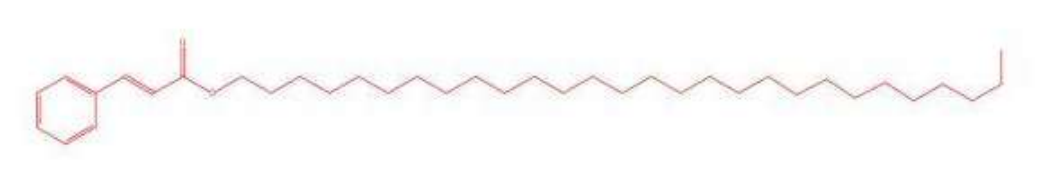
```
Uploading structure file: cinnamic ester
```






```
Node Attributes
Ring Nodes : 1  2  3  4  5  6
```

```
Chain Nodes : 7  8  9  10  11  13
Bond Attributes
Ring Bonds : 1-2  2-3  3-4  4-5  5-6  6-1
Chain Bonds : 5-7  7-8  8-9  9-10  10-11  11-12  13-9
Exact Bonds : 5-7  7-8  8-9
Normalized Bonds : 1-2  2-3  3-4  4-5  5-6  6-1
Exact/Normalized Bonds : 9-10  10-11  11-12  13-9
Markush Attributes
Match Level (ATOM) : 1  2  3  4  5  6
Match Level (CLASS) : 7  8  9  10  11  12  13
Element Count Level (LIMITED) : 1  2  3  4  5  6  7  8  9  10  11  12  13

L1      STRUCTURE UPLOADED

=> s l1 css ful

FULL SEARCH INITIATED 05:33:10 FILE 'REAXYSFILESU'
FULL SCREEN SEARCH COMPLETED -        0 TO ITERATE

     0.0% PROCESSED   49510784 ITERATIONS    187 ANSWERS
SEARCH TIME: 00.01.44

L2          187 SEA CSS FUL L1

=> s l2 and mp/fa.p

       7695407 MP/FA.P
L3          18 L2 AND MP/FA.P

=> d

L3     ANSWER 1 OF 18 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN     49531772   REAXYSFILESU
MF     C37 H64 O2
CMF    C37 H64 O2
LSF    C37H64O2
INCHI  WXOZRCXXCCYWOK-UHFFFAOYSA-N
MW     540.914
MARKREF.CNT 0
REC    1
ED     Entered STN: 20 Mar 2023
       Last updated on STN: 19 Jan 2024
```



```
Melting Point (1)
 Value      | Location             | Ref(s)
 (MP)       | (.LO)                | (REF)
 (Cel)      |                      |
============+======================+============
 69 - 71    | supporting informati | 1
            | on                   |

1. AN 123575571: Journal: Dawurung, Christiana J. et al., Molecules (2023)
Vol. 28, No.2 arn.673
```

2. Keywords (/KW)

In the /KW search field all keywords of the different properties are concentrated. They support searching for a property without knowing the correct property field.

Example 2:
Search for europium - iron compounds with superconductivity information.

```
=> s (eu and fe)/els and superconductivity/kw

         43809 EU/ELS
        353411 FE/ELS
         21029 SUPERCONDUCTIVITY/KW
L1          21 (EU AND FE)/ELS AND SUPERCONDUCTIVITY/KW

=> d

L1     ANSWER 1 OF 21 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN     57000469   REAXYSFILESU
MF     As3 Eu Fe4 P Rb
CMF    As3 Eu Fe4 P Rb
LSF    RbEuFe4As3.25P0.75
INCHI  RYUPIUPCLBCDSR-UHFFFAOYSA-N
MW     727.541
MARKREF.CNT 0
REC    1
ED     Entered STN: 14 Dec 2023
       Last updated on STN: 19 Jan 2024

                        Substance image not available

Electrical Data (2)
 Keyword              | Crit. Temp. | Ref(s)
 (.KW)                | (.CRIT)     | (REF)
                      | (Cel)       |
======================+=============+============
 Superconductivity    | -238.78     | 1
 Superconductive tran |             | 1
 sition temperature   |             |

1. AN 130126585: Journal: Usman, Mohammad et al., Chem. Mater. (2023) Vol.
35, No.20, pp. 8494 - 8501
```

3. Properties (/FA.P)

Example 3:

Search for natural ingredients with spectroscopic information.
All Boolean operators may be used depending on desired precision.
Further option for display: D SPEC shows all available spectroscopic data.

Please note: SET LINE 150 for better readability of property tables.

```
=> SET LINE 150

=> s inp/fa.p and (ms and nmr and ir and uvs)/fa.p

        316789 INP/FA.P
      12305613 MS/FA.P
      14956017 NMR/FA.P
       6564641 IR/FA.P
       1815392 UVS/FA.P
L3       88871 INP/FA.P AND (MS AND NMR AND IR AND UVS)/FA.P

=> d

L3     ANSWER 1 OF 88871 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN     57424697   REAXYSFILESU
CN     euphylonane G
MF     C35 H44 O9
CMF    C35 H44 O9
LSF    C35H44O9
INCHI  UMEABDUVKKGNCL-ILXSNTAKSA-N
MW     608.729
MARKREF.CNT 0
REC    1
ED     Entered STN: 1 Feb 2024
       Last updated on STN: 1 Feb 2024

       Substance image not available

IR spectroscopy (1)
 Keyword         | Solvent           | Location             | Ref(s)
 (.KW)           | (.SOL)            | (.LO)                | (REF)
=================+===================+======================+============
 Bands; Spectrum | neat (no solvent) | supporting informati | 1
                 |                   | on                   |

1. AN 130962458: Journal: Wu, Shu-Qi et al., J. Nat. Prod. (2023)

Mass Spectrometry (1)
 Keyword              | Location             | Ref(s)
 (.KW)                | (.LO)                | (REF)
======================+======================+============
 high resolution mass | supporting informati | 1
  spectrometry (HRMS) | on                   |
 ; electrospray ionis |                      |
 ation (ESI); time-of |                      |
 -flight mass spectra |                      |
  (TOFMS); spectrum   |                      |

1. AN 130962458: Journal: Wu, Shu-Qi et al., J. Nat. Prod. (2023)

NMR spectroscopy (7)
 Keyword              | Nucleus    | Solvent       | Location             | Ref(s)
```

(.KW)	(.NUC)	(.SOL)	(.LO)	(REF)
Chemical shifts; Spectrum	1H	chloroform-d1	supporting information	1
COSY (Correlation Spectroscopy); Spectrum	1H; 1H	chloroform-d1	supporting information	1
NOESY (Nuclear Overhauser Enhanced Spectroscopy); Spectrum	1H; 1H	chloroform-d1	supporting information	1
HSQC (Heteronuclear Single Quantum Coherence); Spectrum	1H; 13C	chloroform-d1	supporting information	1
HMBC (Heteronuclear Multiple Bond Coherence); Spectrum	1H; 13C	chloroform-d1	supporting information	1
Chemical shifts; Spectrum	13C	chloroform-d1	supporting information	1
DEPT (Distorsionless Enhancement by Polarisation Transfer); Spectrum	13C	chloroform-d1	supporting information	1

1. AN 130962458: Journal: Wu, Shu-Qi et al., J. Nat. Prod. (2023)

UV/VIS spectroscopy (1)

Solvent (.SOL)	Ref(s) (REF)
acetonitrile	1

1. AN 130962458: Journal: Wu, Shu-Qi et al., J. Nat. Prod. (2023)

Isolation from Natural Product (1)

Value (INP) (--)	Ref(s) (REF)
whole plants of Euphorbia hylonoma	1

1. AN 130962458: Journal: Wu, Shu-Qi et al., J. Nat. Prod. (2023)

Overview of Reactions

Summary

Finding reactions for a substance – combine, e.g., a structure search with field availability and use QRD for display (see example 7) **=> S L# and RX.ID/FA.RX**

Find preparations of a substance (see example 5) **=> S L# AND PREPARATION/RX.CL**

Use of paragraph proximity (example 4) e.g., to search two substances in one reaction

Reaction data are clearly separated in two parts, reaction identification data and reaction details (same ID with added counter), as shown in the example below (chemical names are shortened).

```
Reaction:
       Reaction ID:                    30015584
       Reactant AN (.RAN):             14292834; 7703552
       Reactant (.RCT):                4-bromo-2-chloro-1-[(1-
                                       methylethyl)oxy]benzene;
                                       bis(pinacol)diborane
       Product AN (.PAN):              21007747
       Product (.PRO):                 2-{3-chloro-4-[(1-methylethyl)oxy]phenyl}-
                                       4,4,5,5-tetramethyl-1,3,2-dioxaborolane
       Reference Count:                7

Reaction Details:
       Reaction RID:                   30015584.1
       Reaction Classification (.CL): Preparation
       Product AN (.PRAN)              21007747
       Reactant AN (.RCAN):            13182466; 4267587
       Solvent AN (.SOLAN):            605365
       Product:                        2-{3-chloro-4-[(1-methylethyl)oxy]phenyl}-
                                       4,4,5,5-tetramethyl-1,3,2-dioxaborolane
       Reagent:                        dichloro(1,1'-
                                       bis(diphenylphosphanyl)ferrocene)palladiu
                                       m(II)*CH2Cl2; potassium carbonate
       Solvent:                        N,N-dimethyl-formamide
       Temperature:                    80 Cel
       Yield:                          11.8 g
       Reference(s):                   35460124: Patent, US 20130012491 A1


       Reaction RID:                   30015584.2
       Reaction Classification (.CL): Preparation
       Reactant AN (.RCAN):            3595449
       Solvent AN (.SOLAN):            605365
       Catalyst AN (.CAAN):            13182466
       Catalyst:                       dichloro(1,1'-
                                       bis(diphenylphosphanyl)ferrocene)palladiu
                                       m(II)*CH2Cl2
       Reagent:                        potassium acetate
       Solvent:                        N,N-dimethyl-formamide
       Temperature:                    20 - 80 Cel
       Reference(s):                   20010910: Patent, WO 2011113309 A1
```

All reactions possessing identical reaction identification data, which means reactions with the same reactants and products, are combined under one Reaction ID. Particular facts of a distinct way to carry out a reaction are given in the reaction details.

Reaction details provide explicit information about reaction conditions. If quoted in the literature, further information such as yield, reagent, catalyst, solvent, time, temperature and reaction type are indexed.

Depending on the aim of investigation, reaction details are classified, e.g., as preparation or chemical behaviour in the reaction classification field (/RX.CL). A reaction is ranked as “preparation” if the investigation focused on the preparative methods. Chemical behavior is assigned, e.g., to data concentrating on thermodynamic or kinetic studies of a reaction. “Multistage” reactions are a special type of preparations where the structures of intermediates are unknown.

```
=> e a/rx.cl
**** START OF FIELD ****
E3           0 --> A/RX.CL
E4     1171799     CHEMICAL BEHAVIOUR/RX.CL
E5      172025     MARKUSH REACTION/RX.CL
E6    10709632     MULTI-STEP REACTION/RX.CL
E7    23762931     PREPARATION/RX.CL
E8     5172426     PREPARATION (HALF REACTION)/RX.CL
**** END OF FIELD ****
```

Reactions - good to know

Please note: The paragraph operator (P) is used to specify that two terms must be in the same information unit, in this case in the same Reaction Identification data.

Example 4:
Combined search for preparation and reactant

```
S  1000/RX.PAN (P) 6831972/RX.RAN
```

To specify that, e.g., “preparation” as a classification occurs in the same reaction document, use (P) proximity.

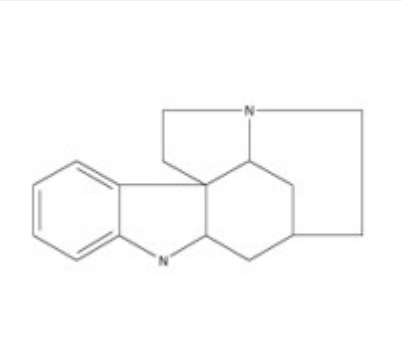
Available Search Fields:

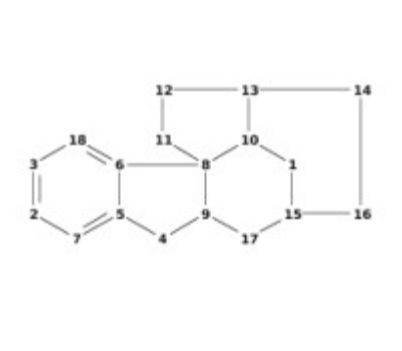
Search Field Code	Long Name	How to Use
RX.ID	Reaction document	RX.ID/FA.RX
PAN	Product Accession Number	/RX.PAN
RAN	Reactant Accession Number	/RX.RAN
CL	Classification	/RX.CL
AAN	All Accession Numbers in reaction document	/RX.AAN
PRO, RCT	Chemical names or molecular formulas of products, reactants	Please use EXPAND!

Example 5:

Search for preparations of substances with condyfolan substructure.

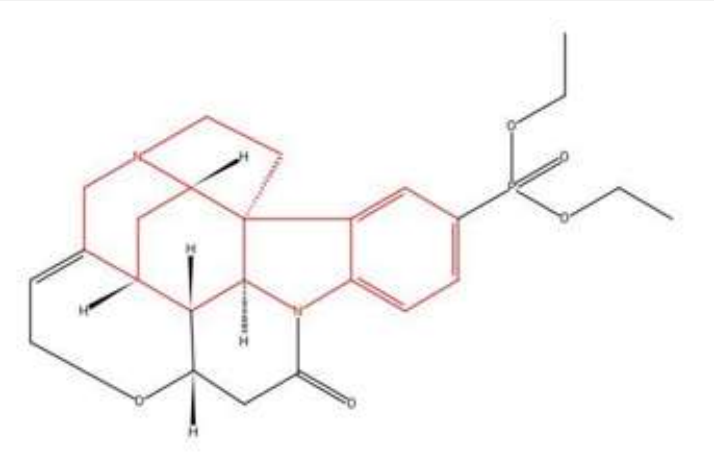
```
Uploading structure file: condyfolan
```





```
Node Attributes
Ring Nodes : 1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18
Bond Attributes
Ring Bonds : 1-15  2-3  3-18  4-5  4-9  5-6  5-7  6-8  6-18  7-2  8-9  8-10
9-17  10-1  10-13  11-8  11-12  12-13  13-14  14-16  15-16  15-17
Normalized Bonds : 2-3  3-18  5-6  5-7  6-18  7-2
Exact/Normalized Bonds : 1-15  4-5  4-9  6-8  8-9  8-10  9-17  10-1  10-13
11-8  11-12  12-13  13-14  14-16  15-16  15-17
Markush Attributes
Match Level (ATOM) : 1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17
18
Element Count Level (LIMITED) : 1  2  3  4  5  6  7  8  9  10  11  12  13  14
15  16  17  18


L1      STRUCTURE UPLOADED

=> s l1 ful

FULL SEARCH INITIATED 02:29:09 FILE 'REAXYSFILESU'
FULL SCREEN SEARCH COMPLETED -        0 TO ITERATE
0.0% PROCESSED   49605936 ITERATIONS              3664 ANSWERS
SEARCH TIME: 00.01.27


L2         3664 SEA SSS FUL L1

=> s l2 and preparation/rx.cl

      23789332 PREPARATION/RX.CL
L3        1413 L2 AND PREPARATION/RX.CL

=> d

L3     ANSWER 1 OF 1413 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN     57408373   REAXYSFILESU
MF     C25 H31 N2 O5 P
```

CMF C25 H31 N2 O5 P
LSF C25H31N2O5P
INCHI IPEGNYNLMRQRQS-XPJHAGJWSA-N
MW 470.505
MARKREF.CNT 0
REC 1
ED Entered STN: 1 Feb 2024
Last updated on STN: 1 Feb 2024



Reaction:

Reaction ID:	65760958
Reactant AN (.RAN):	5412178; 605759
Reactant (.RCT):	2-iodostrychnine; phosphonic acid diethyl ester
Product AN (.PAN):	57408373
Product (.PRO):	C25H31N2O5P
Reference Count:	1

Reaction Details:

Reaction RID:	65760958.1
Reaction Classification (.CL):	Preparation
Product AN (.PRAN)	57408373
Reactant AN (.RCAN):	105690; 16475472; 23015538; 3602276; 57408372; 7085968; 8128145
Solvent AN (.SOLAN):	3587155; 506104
Product:	C25H31N2O5P
Reagent:	2,6-dimethylpyridine;…
Solvent:	water; ethyl acetate
Temperature:	45 Cel
Yield:	65 percent
Reference(s):	130002965: Journal: Navratil, Rafael et al., Green Chem. (2023) Vol. 25, No.23, pp. 9779 - 9794

Example 6:

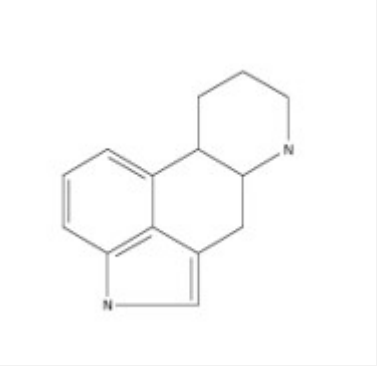
Search for AN 55280523 (anhydropereirine) in all reaction fields with Accession Numbers.

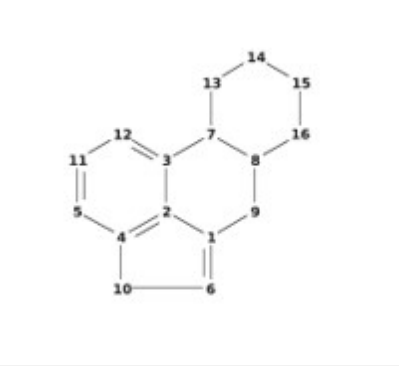
```
=> s 55280523/rx.aan

L5          14 55280523/RX.AAN

Required Accession Number is found in different fields of the reaction document
(two selected examples):

Reaction:
       Reaction ID:                  64122497
       Reactant AN (.RAN):           55280574
       Reactant (.RCT):              C24H19N3O6S
       Product AN (.PAN):            55280523
       Product (.PRO):               (-)-anhydropereirine
       Reference Count:              1
…

Reaction:
       Reaction ID:                  64122148
       Reactant AN (.RAN):           55280523
       Reactant (.RCT):              (-)-anhydropereirine
       Product AN (.PAN):            27897521
       Product (.PRO):               (-)-19,20-dihydrovalparicine
       Reference Count:              1
```

Example 7:

Search for ergoline derivatives (closed substructure search) with reaction information.

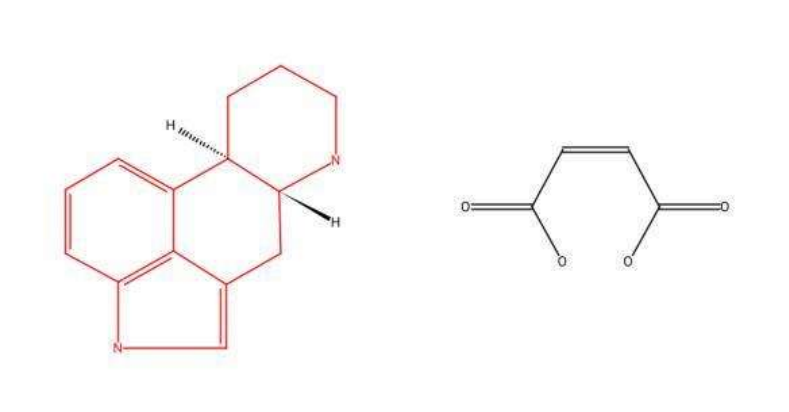
```
Uploading structure file: ergoline
```





```
Node Attributes
Ring Nodes : 1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16
Bond Attributes
Ring Bonds : 1-2  1-6  1-9  2-3  2-4  3-7  3-12  4-5  4-10  5-11  6-10  7-8  7-13  8-9
8-16  11-12  13-14  14-15  15-16
Normalized Bonds : 2-3  2-4  3-12  4-5  5-11  11-12
Exact/Normalized Bonds : 1-2  1-6  1-9  3-7  4-10  6-10  7-8  7-13  8-9  8-16  13-14
14-15  15-16
Markush Attributes
Match Level (ATOM) : 1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16
Element Count Level (LIMITED) : 1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16


L8      STRUCTURE UPLOADED

=> s l8 css ful

FULL SEARCH INITIATED 02:57:06 FILE 'REAXYSFILESU'
FULL SCREEN SEARCH COMPLETED -        0 TO ITERATE

  0.0% PROCESSED   49605936 ITERATIONS        10 ANSWERS
SEARCH TIME: 00.00.46

L9           10 SEA CSS FUL L8


=> s l9 and rx.id/fa.rx

      28414331 RX.ID/FA.RX
L10           2 L9 AND RX.ID/FA.RX

=> d 1-2

L10    ANSWER 1 OF 2 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN     13328795   REAXYSFILESU
CN     ergoline maleate
MF     C4 H4 O4 . C14 H16 N2
CMF    C4 H4 O4; C14 H16 N2
LSF    C4H4O4*C14H16N2
INCHI  UHLMNQPSHNOIPZ-DNOYJIHHSA-N
AINCHI UHLMNQPSHNOIPZ-DOLCSHREDO
```

MW 328.368
MARKREF.CNT 0
REC 2
ED Entered STN: 15 Jul 2020
Last updated on STN: 19 Jan 2024

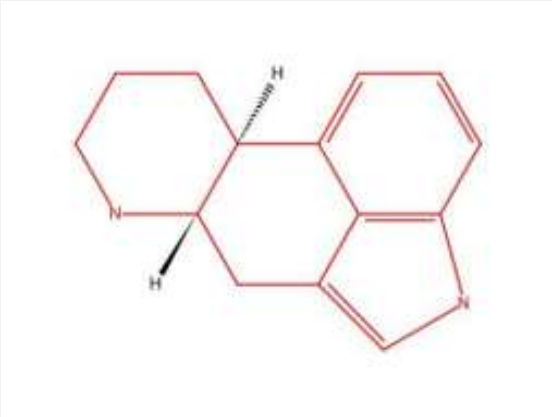


Reaction:
Reaction ID: 25325835
Product AN (.PAN): 13328795
Product (.PRO): ergoline maleate
Reference Count: 2

Reaction Details:
Reaction RID: 25325835.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s): 32797: Patent, US 4197299 A

Reaction RID: 25325835.2
Reaction Classification (.CL): Preparation (half reaction)
Reference(s): 35474: Patent, US 4229450 A

L10 ANSWER 2 OF 2 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN 17738 REAXYSFILESU
CN (i)rac-ergoline; (i)rac-Ergolin;
(6aS,10aS)-4,6,6a,7,8,9,10,10a-Octahydro-indolo[4,3-fg]quinoline
SD heterocyclic
MF C14 H16 N2
CMF C14 H16 N2
LSF C14H16N2
INCHI RHGUXDUPXYFCTE-GWCFXTLKSA-N
AINCHI RHGUXDUPXYFCTE-GWCFXTLKBK
MW 212.294
MARKREF.CNT 0
REC 2
ED Entered STN: 14 Jul 2020
Last updated on STN: 19 Jan 2024



Reaction:

Reaction ID:	22298256
Reactant AN (.RAN):	254518
Reactant (.RCT):	7-nitro-benzo[<i>f]quinoline…
Product AN (.PAN):	17738
Product (.PRO):	<i>rac-ergoline
Reference Count:	1

Reaction Details:

Reaction RID:	22298256.1
Reaction Classification (.CL):	Multi-step reaction
Reactant AN (.RCAN):	11342940; 3647881; 4933679
Reagent:	sodium hydroxide; sodium; iron(II) sulfate
Reference(s):	705489: Journal: Jacobs et al., J. Biol.Chem. (1937) Vol. 120, 141,150p.

Reaction:

Reaction ID:	263473
Reactant AN (.RAN):	183432; 969148
Reactant (.RCT):	4<i>H-indolo[4,3-<i>fg]quinolin-5-one; butan-1-ol
Product AN (.PAN):	17738; 20981
Product (.PRO):	<i>rac-ergoline; (7-amino-1,2,3,4,4a,5,6,10b-octahydro-benzo[<i>f]quinolin-6-yl)-methanol
Reference Count:	1

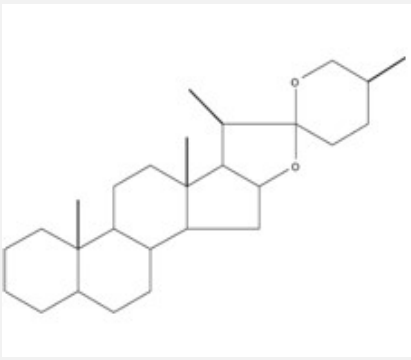
Reaction Details:

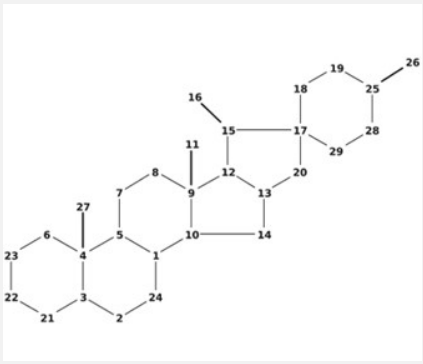
Reaction RID:	263473.1
Reaction Classification (.CL):	Preparation
Reactant AN (.RCAN):	3647881
Reagent:	sodium
Reference(s):	705489: Journal: Jacobs et al., J. Biol. Chem. (1937) Vol. 120, 141,150p.

Example 8:

Search for spirostane substructures that are listed as a product in reaction documents.
Use ANALYSE (for up to 50,000 accession numbers) and combine with /RX.PAN to restrict to reaction product.

```
Uploading structure file: spirostane
```






```
Node Attributes
Ring Nodes : 1  2  3  4  5  6  7  8  9  10  12  13  14  15  17  18  19  20  21  22  23  24
25  28  29
Chain Nodes : 11  16  26  27
Bond Attributes
Ring Bonds : 1-10  1-24  2-3  2-24  3-4  3-21  4-5  4-6  5-1  5-7  7-8  8-9  9-10  9-12
10-14  12-13  12-15  13-14  13-20  15-17  17-18  17-20  17-29  18-19  19-25  21-22  22-23
23-6  25-28  28-29
Chain Bonds : 4-27  9-11  15-16  25-26
Exact Bonds : 4-27  9-11  15-16  25-26
Exact/Normalized Bonds : 1-10  1-24  2-3  2-24  3-4  3-21  4-5  4-6  5-1  5-7  7-8  8-9
9-10  9-12  10-14  12-13  12-15  13-14  13-20  15-17  17-18  17-20  17-29  18-19  19-25
21-22  22-23  23-6  25-28  28-29
Markush Attributes
Match Level (ATOM) : 1  2  3  4  5  6  7  8  9  10  12  13  14  15  17  18  19  20  21  22
23  24  25  28  29
Match Level (CLASS) : 11  16  26  27
Element Count Level (LIMITED) : 1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17
18  19  20  21  22  23  24  25  26  27  28  29

L1      STRUCTURE UPLOADED

=> s l1 ful

FULL SEARCH INITIATED 04:34:39 FILE 'REAXYSFILESU'
FULL SCREEN SEARCH COMPLETED -        0 TO ITERATE

0.0% PROCESSED   49918784 ITERATIONS             5765 ANSWERS
SEARCH TIME: 00.00.31

L2         5765 SEA SSS FUL L1

=> ana l2 1-

L3          ANALYZE L2 1- AN :    5765 TERMS
```

```
=> s l3/rx.pan

L5        4329 L3/RX.PAN

=> d 4302

L5     ANSWER 4302 OF 4329 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN     45102   REAXYSFILESU
RN     547-01-3
CN     tokorogenin
SD     heterocyclic
MF     C27 H44 O5
CMF    C27 H44 O5
LSF    C27H44O5
INCHI  SRTGQBIWSBCVSM-RXWDRLOESA-N
AINCHI SRTGQBIWSBCVSM-RXWDRLOEBC
MW     448.643
MARKREF.CNT 0
REC    12
ED     Entered STN: 15 Jul 2020
       Last updated on STN: 19 Jan 2024

                     Structure image

Reaction:
       Reaction ID:                   5180294
       Reactant AN (.RAN):            8307197
       Reactant (.RCT):               arundinoside A
       Product AN (.PAN):             45102
       Product (.PRO):                tokorogenin
       Reference Count:               1


Reaction Details:
       Reaction RID:                  5180294.1
       Reaction Classification (.CL): Preparation
       Reactant AN (.RCAN):           1098214
       Reagent:                       hydrogenchloride
       Time:                          6 s
       Reference(s):                  6172139: Journal: Tandon, Mamta et al., J.
Indian
                                      Chem. Soc. (1997) Vol. 74,
                                      No.1, pp. 56 - 58
```

Property Glossary
(Properties in Alphabetical Order)

Acoustic Properties (SOUND)
This field contains information about:
- Velocity of sound
- Sound absorption
- Acoustic relaxation
- Ultrasonic properties
- Ultrasonic velocity
- Hypersonic velocity
- Ultrasonic absorption
- Hypersonic absorption

Adsorption (ADSM)
This field describes a multi-component system.
The field Adsorption Description (/ADSM) contains keywords from the following list of controlled terms:
- Adsorption
- Adsorption isotherm
- Chemisorption
- Enthalpy of adsorption
- Further physical properties of the adsorbed molecule
- Desorption
- Adsorption and desorption isotherms
- Rate of adsorption
- Desorption isotherm(s)
- Rate of desorption

Association (ASSM)
This field describes a multi-component system.
The field Association Description (/ASSM) contains keywords from the following list of controlled terms:
- Association with compound
- Stability constant
- Enthalpy of association
- Dipole moment of the complex
- Spectrum of the complex
- Further physical properties of the complex
- Exciplex formation
- IR spectrum of the complex
- NMR spectrum of the complex
- UV/VIS spectrum of the complex

Autoignition (AIT)
The autoignition temperature or self-ignition temperature of a substance is the lowest temperature at which the substance spontaneously ignites in a normal atmosphere without an external source of ignition, such as a flame or a spark. This is the temperature required to supply the activation energy needed for combustion. Also known as the spontaneous ignition temperature, minimum ignition temperature, ignition temperature, and the kindling point.

Azeotropes (AZE)
This field describes a multi-component system.
An azeotrope is a multi-component solution in which the composition of liquid and vapor phases are equal; therefore, there is no change in composition upon boiling.
The Azeotrope field contains the azeotrope of the title compound with another substance.

Boiling Point (BP)
The boiling point is the temperature at which the vapor pressure of a liquid equals the external pressure. The normal boiling point is the temperature at which the vapor pressure equals the normal atmospheric pressure.

Boundary Surface Phenomena (BSPM)
This field describes a multi-component system.
The field Boundary Surface Phenomena Description (BSPM) contains keywords from the following list of controlled terms:

- Surface tension
- Surface potential
- Surface moment
- Pressure-surface isotherm
- Spreading pressure
- Interfacial tension
- Contact angle with compound
- Boundary surface phenomena
- Micellar weight
- Further surface properties

Bulk Viscosity (BV)
Bulk viscosity is the force per unit area required to maintain unit difference of velocity between two layers 1 cm apart. The values are given at the measurement temperatures and can be found in the associated parameter field code /BV.T.

Circular Dichroism (CDIC)
Optically active compounds absorb left and right polarized light unequally. When linearly polarized incident light passing through a substance becomes elliptically polarized the phenomenon is known as circular dichroism. The wavelength range over which this phenomenon has been measured is stored in the CDIC field.

Complex Phase Equilibria (CPEM)
This field contains information about:

- Solid-vapor phase equilibrium
- Liquid-solid-vapor phase diagram
- Liquid-solid-vapor phase equilibrium
- Triple point
- Quadruple point
- Phase equilibrium

Compressibility (CMP)
This field contains information about:

- Adiabatic compressibility
- Isothermal compressibility

Conformation (CNF)
This field contains information about:

- Energy barrier
- Energy difference between conformers
- Equilibrium constant
- Equilibrium data
- Kinetics

Critical Density (CRD)
The Critical Density field contains the numerical value for the density of a substance measured at its critical temperature and pressure.

Critical Micelle Concentration (CMC)
This field describes a multi-component system.
The critical micelle concentration is the concentration at which micelles begin to form in a system comprising solvent(s), surfactant(s), possibly other solutes and a defined physical environment. You can search for the associated temperature and solvent information in the parameter fields /CMC.T and /CMC.SOL.

Crystal Phase Transition Point (CPTP)
The Crystal Phase Transition Point is the temperature at which two crystal phases (triclinic, monoclinic, rhombic, cubic, tetragonal, hexagonal) are in equilibrium. The Crystal Phase Transition Point field contains the temperature at which two crystal phases are in the equilibrium for substances. The Crystal Phase Transition Point is a numeric search field. It is range searchable.

Critical Pressure (CRP)
The critical pressure is the minimum pressure required for liquefying a gas at its critical temperature. The Critical Pressure field contains the value of the critical pressure for the substance.

Critical Temperature (CRT)
The critical temperature is the temperature above which a gas cannot be liquefied by pressure. The Critical Temperature field contains the values of the critical temperature for the substance.

Critical Volume (CRV)
The Critical Volume field contains values for the molar volumes of substances measured at their critical pressures and critical temperatures

Cross-Section (XS)
This field contains information about:

- Photoionization cross-section
- Electron ionization cross-section
- Proton ionization cross-section
- Ionization cross-section
- Collision cross-section

Crystal Phase (CRYPH)
This field contains information about:

- Rate of crystallization
- Polymorphism
- Rate of transition
- Crystal habit
- Crystal growth
- Crystal morphology
- Crystal structure determination (crystal lattice parameters)
- Interplanar spacing
- Association in the solid state
- Solid state structure properties
- Melting pressure
- Freezing point
- Glass transition temperature
- Phase diagram
- Long spacing
- Reorientation in the solid state
- Spin polarization
- Nuclear spin conversion
- Structure of the solid
- Dimensions of the unit cell

Crystal Property Description (CPD)
The Crystal Property Description field contains terms that give a qualitative description of the outward appearance of crystalline materials such as the color of the crystal and its shape.

Crystal Space Group (CSG)
The Space Group field contains information on the different crystal space groups using the relevant terms.

Crystal System (CSYS)
The Crystal System field contains information on the seven crystal classes: cubic, hexagonal, trigonal, tetragonal, monoclinic, triclinic and rhombic. You can search in the Crystal System field using the class name of the crystal system of interest.

Decomposition Point (DP)
The decomposition point is the temperature at which a substance undergoes thermal decomposition at atmospheric pressure.

Density of the Liquid (DEN)
Density is defined as mass per unit volume at a particular temperature and pressure. The Density field contains values for the crystal density at 1 atm or below and liquid density at 1 atm when below normal boiling point, at saturation pressure at and above normal boiling point. Because the density varies with the temperature, you can search for the associated measurement temperature and reference temperature in the parameter fields /DEN.T and /DEN.RT.

Chemical Derivative (CDER)
Characterization derivatives and addition compounds (salts, complexes, adducts, associations, clathrates) are recorded as individual compounds with all their data. In other cases, the Derivative field CDER contains chemical names and additional information about derivatives of the cited substance (e.g., salt names, salt molecular formulae, and melting point of derivatives). The Accession Number of the derivative can be found in the parameter field /CDER.AN.

Examples for substances used for characterization:
- Picrates
- Phenylhydrazones
- Semicarbazones
- Acetyl derivatives
- Benzoyl derivatives
- Oximes

Dielectric Constant (DIC)
The dielectric constant is the ratio of the capacity of a condenser with that substance as the dielectric medium to the capacity of the same condenser in a vacuum. The values of the constant are given at specified temperatures and frequencies. You can search for the associated frequency and temperature in the parameter fields /DIC.F and /DIC.T.

Static Dielectric Constant (SDIC)
For a given substance the static dielectric constant is the ratio of the capacity of a condenser with that substance as the dielectric medium to the capacity of the same condenser with a vacuum as the dielectric medium. The dielectric constant is a function of temperature and frequency at which the alternating electric field varies.

The static dielectric constant is the dielectric constant at frequencies low enough that the equilibrium is maintained as the electric field varies. The values of the constant are given at specified temperatures. You can search for the associated temperature in the parameter fields /SDIC.T.

Electrical Moment (EM)
This field contains information about:
- Bond moment
- Dipole moment
- Quadrupole moment
- Hexadecapole moment
- Octopole moment

Dissociation Exponent (DE)
The dissociation exponent is defined as the logarithm (base 10) of the reciprocal of the equilibrium constant. The Dissociation Exponent field contains the values for the dissociation exponents (pKa for acids, pKb for bases). You can search for the associated information about dissociation group, temperature, solvent, method and type using the parameter field codes /DE.GRP, /DE.T, /DE.SOL, /DE.MET and /DE.TYP.

Dynamic Viscosity (DV)
Dynamic viscosity is the ratio of the shearing stress to the rate of shear. The Dynamic Viscosity field contains the values for the dynamic viscosity of substances given at specified temperatures. You can search for this associated information using the parameter field code DV.T.

Electrical data (ELE)
This field contains information about:

- Angle of dielectric loss
- Critical frequency (or wavelength)
- Dielectric anisotropy
- Dielectric increment
- Dielectric loss
- Dielectric relaxation time
- Dielectric saturation
- Relaxation frequency
- Cole-Cole diagram
- Piezoelectricity
- Thermoelectricity
- Photoelectricity (Becquerel effect)
- Electrical conductivity
- Photoconductivity
- Dielectric strength
- Electrical properties
- Photovoltaic effect

Electrical Data (EDM)
This field describes a multi-component system.
The information stored in this field corresponds to the information stored in the field ELE.

Electrical Polarizability (ELP)
This fields contains information about the following topics:

- Atom polarization
- Electron polarization
- Hyperpolarizability
- Molar polarization
- Optical anisotropy
- Polarizability

Electrochemical Behavior (ELCB)
This topic contains information about:

- Autoprotolysis
- Enthalpy of dissociation (electrolytic) / protonation
- Kinetics of dissociation (electrolytic) / protonation
- Enthalpy of neutralization
- Proton affinity
- Electrolytic dissociation / protonation equilibrium
- Thermodynamic parameters for autoprotolysis
- Thermodynamic parameters for dissociation / protonation

- Volume change on dissociation
- Enthalpy of deprotonation
- Acidity
- Basicity
- Protonation
- Deprotonation
- pK(R+)
- pH of aqueous solutions
- Stability constant
- Electrochemical properties
- Polarography
- Degree of dissociation

Electrochemical Data (ELCH)
The electrochemical cell potential field contains the values for cells using substances of the file as electrode material, as electrolyte or as compound of the electrolyte. The electrochemical cell potential field is linked to the associated temperature. A pair of electrodes dipping into an ionic medium called electrolyte (solid, liquid or gas) and connected by an external electric conductor constitutes an electrochemical cell.

Electrochemical Characteristics (POT)
The field Electrochemical Characteristics Description (/POT) contains keywords from the following list of controlled terms:
- Cyclic voltammetry
- Oxidation potential
- Polarographic current/voltage curve
- Polarographic half-wave potential
- Redox potential
- Reduction potential
- Voltammetry
- Photo-electrochemical half-wave potential

Electrolytic Conductivity (ELYC)
The molar (specific) electrolytic conductivity is the reciprocal of the resistivity, per mole (gram) per unit volume of solution. The equivalent electrolytic conductivity is the molar electrolytic conductivity per number of equivalents.

Electron Binding (CIP)
This field contains information about:
- Electron affinity
- Core IP

Energy Barriers (EBC)
The Energy Barriers field contains the values for the amount of energy required to convert one conformation of a molecule to another where both conformations represent energy minima. Conformations are defined as spatial arrangements of the atoms in a molecule, which can be interconverted by rotation about a single bond. You can search for the associated information about the bond type using the parameter field code /EBC.TYP.

Energy Data (ENEM)
This field describes a multi-component system.
The field Energy Data Description (/ENEM) contains keywords from the following list of controlled terms:
- Enthalpy of solution
- Enthalpy of mixing
- Enthalpy of dilution
- Enthalpy of evaporation
- Heat capacity of mixtures
- Enthalpy of mixtures
- Entropy of mixtures

- Excess thermochemical parameter
- Partial molar enthalpy of mixing
- Heat capacity Cp
- Heat capacity Cv
- Excess heat capacity Cp
- Molar excess Gibbs free energy

Dissociation Energy (EDIS)
The dissociation energy is defined as the energy required to break a specific bond in one mol of a compound to produce two fragments. You can search for the associated information about the bond type using the parameter field code /EDIS.TYP.

Enthalpy of Combustion (HCOM)
The enthalpy of combustion is the change in enthalpy, which occurs when one mol of a compound reacts completely with an excess of oxygen at atmospheric pressure and at room temperature, the products being in their natural physical state under these conditions. The values are given at specified temperatures and pressures. You can search for this associated information using the parameter field codes /HCOM.T and /HCOM.P, respectively.

Enthalpy of Formation (HFOR)
The enthalpy of formation is the change in enthalpy, which occurs when one mol of the compound is formed from its elements each being in its natural state at ordinary temperature and pressure. The values are given at specific temperatures and pressures and can be found in the parameter field codes /HFOR.T and /HFOR.P, respectively.

Enthalpy of Fusion (HFUS)
The enthalpy of fusion is the change in enthalpy which occurs when one mol of a solid is converted to a liquid at a constant pressure.

Enthalpies of Other Phase Transitions (HPT)
The energy required to convert a compound from one phase to another.

Enthalpy of Hydrogenation (HHDG)
Enthalpy of hydrogenation is defined as the change in enthalpy which occurs when one mol of an unsaturated compound reacts with an excess of hydrogen to become fully saturated at atmospheric pressure and room temperature. The values are given at specified temperatures. This field may be linked to associated chemical name or AN of the saturated compound. You can search for this associated information using the parameter field codes /HHDG.AN, /HHDG.CN and /HHDG.T.

Enthalpy of Sublimation (HSB)
Sublimation is defined as the direct conversion of a solid into a gas at constant temperature and pressure. The enthalpy of sublimation is the change in enthalpy which occurs when one mol of a substance sublimes at a specified temperature and pressure. The values for this field are given at the sublimation temperature.

Enthalpy of Vaporization (HVAP)
The enthalpy of vaporization is the enthalpy change which occurs when one mol of a liquid is converted to a vapor at a constant pressure. The values in this search field are cited at specified temperatures and pressures. You can search for this associated information using the parameter field codes /HVP.T and /HVP.P. If a temperature range has been given in the literature, the average value has been stored.

ESR Spectroscopy (ESR)
The field ESR Description (ESR) contains keywords from a list of controlled terms:
- Spectrum
- Signals
- ENDOR (electron-nuclear double resonance)
- g-factor
- ESR linewidth
- ESR second moment

- Electron spin-lattice relaxation time
- Electron spin-spin relaxation time
- 1H-electron Overhauser effect
- CIDEP (chemically induced dynamic electron polarization)
- ELDOR (electron-electron double resonance)
- ESR
- ESR-hyperfine coupling constants
- Triplet state ESR spectrum
- Triplet state ESR
- Triplet state ESR g-factor
- Triplet state ESR hyperfine coupling constant(s)
- Triplet state ESR zero-field splitting parameter(s)

Explosion Limits (EL)
The explosive range is the range between the lowest explosive limit (LEL) and the upper explosive limit (UEL).

- The LEL is the lowest concentration of vapor in air which will burn or explode upon contact with a source of ignition. Below the LEL, the mixture is too lean (i.e. there is insufficient fuel).
- The UEL is the highest concentration of vapor in air which will burn or explode upon contact with a source of ignition. Above the UEL, the mixture is too rich to burn (i.e. there is insufficient oxygen).

The LEL and UEL are usually indicated by the percentage by volume of vapor in air.

Flash Point (FP)
This is the lowest temperature of the liquid at which it gives off enough vapor to form an ignitable mixture of vapor and air immediately above the liquid surface. A liquid is classified as flammable or combustible depending on its flash point. A flammable liquid has a flash point below 37.8 C while a combustible liquid has a flash point greater than 37.8 C.

Phosphorescence Spectroscopy (PHOS)
The field Phosphorescence Description (PHOS) contains keywords from a list of controlled terms:

- Spectrum
- Maxima
- Phosphorescence lifetime
- Phosphorescence decay kinetics
- Phosphorescence quenching
- Degree of polarization of phosphorescence
- Excimer phosphorescence
- Delayed phosphorescence
- Triplet state energy
- Triplet state quantum yield
- Triplet state lifetime
- Triplet state decay kinetics
- Triplet state quenching
- Triplet state sublevel studies
- Energy transfer from triplet state
- Phosphorescence excitation spectrum
- Phosphorescence quantum yield
- Phosphorescence

Further Information (FINFO)
This field contains references for rarely reported physical and chemical properties.
Examples are:

- Behavior as catalyst
- Behavior as inhibitor
- Colloid chemical behavior

- Ecological data
- Health protection
- Occurrence in nature
- Polymerization
- Reaction of compound surface
- Reaction with substance classes
- Solvation / hydration

Further Information FINFO, FINFO1-3 are a kind of collection pool for rarely examined properties, the added numbers are for technical reasons (not to be confused with category FURTHER PROPERTIES).

Gas Phase (GP)
This field contains information about:
- Fugacity
- Rotational correlation function of the gas
- Neutron scattering of the gas
- Association in the gas phase

Heat Capacity Cp (CP)
The molar heat capacity at constant pressure is defined as the quantity of heat necessary to raise the temperature of 1 mol of the substance 1 degree at constant pressure. The Values are given at specified temperatures. The Heat Capacity CP field contains calorimetric determined values (see also Cp0). You can search for the associated information about the temperature using the parameter field code /CP.T.

Heat Capacity Cp0 (CP0)
The molar heat capacity CP0 is defined as the quantity of heat necessary to raise the temperature of 1 mol of the ideal gas 1 degree at constant pressure. The Heat Capacity CP0 field contains values for ideal gases obtained from statistical thermodynamic calculations (see also CP). You can search for the associated information about the temperature using the parameter field code /CP0.T.

Heat Capacity Cv (CV)
The molar heat capacity CV is defined as the quantity of heat necessary to raise the temperature of 1 mol of the substance 1 degree at constant volume. You can search for the associated information about the temperature using the parameter field code /CV.T.

Henry Constant (HNC)
This field describes a multi-component system.
The Henry constant is the ratio of the concentration of a chemical substance in air to the concentration in an aqueous solution at equilibrium. It can be used as a qualitative measure about the volatility of the substance and its whereabouts in nature. You can search for the value of the constant or its common logarithm. Information on the related temperature and solvent is given in the parameter fields /HNC.T and /HNC.SOL.

IR Spectroscopy (IR)
The field IR Description (IR) contains keywords from a list of controlled terms:
- Spectrum
- Bands
- Fine structure of IR bands
- Intensity of IR bands
- Polarization of IR bands
- Reflection spectrum
- Far IR spectrum
- Near IR spectrum
- Far IR bands
- Near IR bands
- Intensity of far IR bands

- Intensity of near IR bands
- Intensity of rotational lines of IR bands
- Linewidth of IR bands
- Linewidth of rotational lines of IR bands
- IR second moment
- IR-radiofrequency double resonance
- IR-microwave double resonance
- Vibrational relaxation
- Vibrational energy transfer
- Overtone spectrum
- Anisotropy of IR bands
- Fermi resonance
- IR

Interatomic Distances and Angles (IDA)
This field contains information about
- Electron distribution
- Interatomic distances and angles

Ionization Potential (IP)
The ionization potential is defined as the energy per unit charge required to completely removing an electron from an atom or molecule to an infinite distance. The Ionization Potential search field contains the energy values and measurement methods. You can search for the associated information using the parameter field code /IP.MET.

Isoelectric Point (IEP)
The isoelectric point is defined as the pH value at which a substance in a solution is electrically neutral.

Isolation from Natural Product (INP)
The Isolation from Natural Product field contains names of the source in nature (plant, fungus, animal, etc.) or an industrial grade natural product from which compounds have been isolated. Sources are only recorded when a compound has been isolated. The identification of well-known compounds by instrumental methods (e.g., GLC, TLC) as components of natural or synthetic products is not recorded here (e.g., the identification of pentan-2-one in tobacco smoke or limonene in the ethereal oils of a rare plant or saccharose as a component of a tree-bark extract). Terms do not belong to a controlled vocabulary, specific names (e.g., the systematic name of the plant or animal) are used when they are available.

Kinematic Viscosity (KV)
Kinematic viscosity is a coefficient defined as the ratio of the dynamic viscosity of a fluid to its density. The values are given at specified temperatures. These temperatures can be found in the associated parameter field code /KV.T.
Liquid Phase (LQPH)
This field contains information about:
- Rate of evaporation
- Supercoolability
- Structure of the liquid
- Radial distribution function
- Association in the liquid state
- Self-association in solution
- Relaxation time for reorientation
- Rotational correlation time
- Liquid-crystalline properties
- Rotational correlation function of the liquid
- Correlation function of the liquid
- Order parameter
- Liquid-crystalline transition temperatures

Liquid/Liquid Systems (LLSM)
This field describes a multi-component system.
The field Liquid/Liquid Systems Description (/LLSM) contains keywords from the following list of controlled terms:

- Liquid/liquid phase diagram
- Solution equilibrium
- Critical solution temperature
- Temperature of separation
- Equilibrium of liquid phases
- Distribution between solvent 1 + 2
- Solubility diagram
- Critical mixing temperature(s)
- Critical demixing temperature(s)

Liquid/Solid Systems (LSSM)
This field describes a multi-component system.
The field Liquid/Solid Systems Description (/LSSM) contains keywords from the following list of controlled terms:

- Liquid/solid phase diagram
- Melting diagram
- Solidification diagram
- Solidification points of mixtures
- Eutectic
- Liquid-solid phase equilibrium
- Melting points
- Glass transition temperature(s)
- Phase transition temperature(s)

Liquid/Vapor Systems LVSM)
This field describes a multi-component system.
The field Liquid/Vapor Systems Description (/LVSM) contains keywords from the following list of controlled terms:

- Liquid/vapor phase diagram
- Liquid/vapor equilibrium
- Boiling point diagram
- Boiling points of mixtures
- Vapor pressure diagram for the mixture
- Partial pressures of the components
- Critical data for mixtures
- Activity coefficients of the components in the mixture
- Vapor pressure
- Tricritical point
- Critical temperature
- Critical pressure
- Critical density
- Critical volume
- Fugacities

Luminescence Spectroscopy (LUM)
The field Luminescence Description (LUM) contains keywords from a list of controlled terms:

- Emission spectrum in the infrared region
- Radioluminescence
- Sonoluminescence
- Triboluminescence
- Thermoluminescence
- Electroluminescence
- Lasing properties

- Luminescence lifetime
- Luminescence quenching
- Degree of depolarization of luminescence
- Luminescence quantum yield
- Luminescence
- UV/VIS emission spectrum
- UV/VIS emission
- X-ray emission spectrum
- X-ray emission cross-section
- X-ray emission quantum yield
- Luminescence spectrum

Magnetic Data (MAG)
This field contains information about:
- Anisotropy of magnetic susceptibility
- Magnetic moment
- Magnetic properties
- Paramagnetism
- Volume susceptibility
- Rotational magnetic moment

Magnetic Susceptibility (MSUS)
Magnetic susceptibility is the ratio of magnetization to field strength.

Mass Spectrometry (MS)
This field contains keywords from the following list of controlled terms:
- Spectrum
- Chemical ionization (CI)
- Collisional activation
- Electron impact (EI)
- Electrohydrodynamic ionization
- Fast atom bombardment (FAB)
- Field desorption
- Field ionization
- Fragmentation pattern
- High frequency spark
- Hydrogen and carbon scrambling
- Ion kinetic energy (spectrum) (IKE(S))
- Ion current profiles
- Laser desorption
- Metastable ions
- Mass ion kinetic energy (MIKE)
- Negative ion spectroscopy
- Negative secondary ions
- Positive secondary ions
- Charge exchange with rare gas ions
- Collision-induced dissociation
- Doubly charged ions
- Ion-cyclotron resonance
- Ion impact
- Negative chemical ionization
- Neutral impact
- Penning ionization
- Photoelectron-photoion coincidence

- Photoionization
- Secondary ions
- Charge exchange with negative ions
- Neutral fragments
- Surface ionization
- Single ion monitoring (SIMS)
- Liquid secondary ion mass spectrometry (LSIMS)
- Neutralization-reionization mass spectrometry (NRMS)
- Desorption chemical ionization (DCI)
- Time-of-flight mass spectra (TOFMS)
- Multiphoton ionization (MPI)
- Resonance enhanced multiphoton ionization (REMPI)
- Direct electron ionization (DEI)
- Tandem mass spectrometry
- Collisionally activated dissociation (CAD)
- Appearance potentials
- Charge exchange with positive ions

Mechanical and Physical Property (MECM)
This field describes a multi-component system.
The field Mechanical & Physical Properties Description (/MECM) contains keywords from the following list of controlled terms:

- Volume change on mixing
- Partial molal volume
- PVT Relationship
- Virial coefficients
- Adiabatic compressibility
- Isothermal compressibility
- Excess partial molal volume
- Apparent molal volume
- Apparent specific volume
- Second virial coefficient(s) of the equation of state
- Third virial coefficient(s) of the equation of state
- Fourth virial coefficient(s) of the equation of state
- Ultrasonic velocity
- Hypersonic velocity
- Ultrasonic absorption
- Hypersonic absorption
- Acoustic relaxation time

Mechanical Properties (MEC)
This field contains information about:

- Specific volume
- Volume change on melting
- PVT relationship
- Virial coefficients of the equation of state
- Internal pressure
- Elasticity constants
- Compressibility
- Viscosity
- Molar volume
- Second virial coefficient of the equation of state
- Third virial coefficient of the equation of state
- Fourth virial coefficient of the equation of state

Melting Point (MP)
The melting or freezing point of a pure substance is the temperature at which its crystals are in equilibrium with the liquid phase at atmospheric temperature. You can search for the associated information about e.g., the solvent from which the material whose melting point is mentioned was crystallized using the parameter field code /MP.SOL.

Molecular Deformation (DFM)
This field contains information about:

- Fundamental vibrations
- Force constants
- Rotational constants
- Centrifugal distortion constant(s)
- Coriolis coupling constant(s)

Mutarotation (MUT)
Mutarotation is a change in optical rotation that takes place with time in solutions prepared freshly from optically active substances as a result of the reversible conversion of one isomeric form to another. The values are given at a specified wavelength.

NMR Spectroscopy (NMR)
The NMR Spectrum parameter fields are present when the publication contained individual chemical shift values from the NMR spectra for the substances. The field NMR Description (NMR) contains keywords from the following list of controlled terms:

- Spectrum
- Chemical shifts
- Dynamic NMR
- INDOR
- NMR with shift reagents
- Linewidth of NMR absorption
- NMR in liquid-crystal phase
- NOE
- Second moment of NMR absorption
- Spin-lattice relaxation time (T1)
- Spin-spin relaxation time (T2)
- 2D-NMR
- 3D-NMR
- Aromatic solvent induced shifts
- Radical contact shifts
- Double resonance
- Spin-rotation constant
- 1H-electron double resonance
- CIDNP
- NMR
- Spin-spin coupling constants

NQR Spectroscopy (NQR)
The field NQR Description (NQR) contains keywords from a list of controlled terms:

- Nuclear quadrupole resonance
- Nuclear quadrupole coupling constants
- Pure NQR

Optical Data (ODM)
This field describes a multi-component system.
It contains information such as Kerr constant and other optical data.

Optical Rotatory Dispersion (ORD)
Optical rotatory dispersion is defined as the variation in optical rotation with the wavelength of light. The wavelength range over which this phenomenon has been measured is stored in the ORD field.

Optical Rotatory Power (ORP)
The optical rotatory power is the ability of a dissymmetric substance to refract and absorb right- and left-polarized light to different extents. This results in continuous rotation of the plane of polarization.

Optics (OPT)
This field contains information about:

- Crystal refractive indices
- Natural birefringence
- Mechanical birefringence
- Magnetic birefringence (Cotton-Mouton effect)
- Electric birefringence (Kerr effect)
- Diffraction
- Reflection
- Rayleigh scattering
- Degree of depolarization of Rayleigh scattering
- Iso- & anisotropic components of Rayleigh scattering
- Plain curve
- Cotton Effect (abnormal curve)
- Magnetorotation
- Magnetic circular dichroism
- Thermochromism
- Photochromism
- Linear dichroism
- Mutarotation coefficient
- Optical properties
- Rayleigh-Brillouin scattering
- Verdet constant
- Flow birefringence

Other Spectroscopic Methods (OSM)
This field contains information about:

- Photoelectron spectrum
- ESCA
- Moessbauer effect
- Electronic state studies
- Electron impact spectrum
- Auger electron spectrum
- Multiple resonance studies

Other Thermochemical Data (OTHE)
This field contains information about:

- Cryoscopic constant
- Ebullioscopic constant
- Enthalpy
- Heat of combustion at constant volume
- Enthalpy of self-association
- Thermodynamic properties
- Heat capacity
- Entropy
- Heat capacity ratio Cp/Cv
- Gibbs free energy

Partition octan-1-ol/water (POW)
This field describes a multi-component system.
The partition coefficient constant Pow describes the equilibrium distribution of a substance between n-octanol and water phases. The distribution coefficient is the quotient of two concentrations and is usually given in the form of the common logarithm (log POW). You can search for both values POW and log POW. Information on the related temperature is given in the parameter field POW.T.

Patent Specific Data (PSD)
This field contain information on prophetic substances, related Markush structures and location in patent.

Fluorescence Spectroscopy (FLUS)
The field Fluorescence Description (FLU) contains keywords from a list of controlled terms:

- Spectrum
- Maxima
- Fluorescence emission cross-section
- Fluorescence quantum yield
- Fluorescence lifetime
- Fluorescence decay kinetics
- Fluorescence self-quenching
- Fluorescence concentration quenching
- Fluorescence quenching
- Degree of polarization of fluorescence
- Excimer fluorescence
- Delayed fluorescence
- Intersystem crossing [singlet->triplet]
- Energy transfer from singlet state
- Fluorescence excitation spectrum
- Fluorescence intensity
- Fluorescence

Purification (PUR)
The Purification field contains words and phrases that describe the method of purification of a substance.
Comments on the purification of a compound are only accepted when the work, or a large section of it, contains unusual purification methods for the compound in question. Natural occurrence and isolation from natural products are entered under /INP (Isolation from Natural Products). The resolution of racemates does not count as an independent preparation. This is entered under the Description of the preparation of the antipodes (via the racemate) as a method of purification.

Quantum Chemical Calculations (QCC)
The quantum chemical calculations search field refers to quantum chemical calculations performed for a substance. The calculated properties are available in this field together with a classification of the corresponding quantum chemical method of calculation /QCC.MET.

Raman Spectroscopy (RAS)
The field Raman Description (RAS) contains keywords from a list of controlled terms:

- Spectrum
- Bands
- Degree of depolarization of Raman bands
- Hyper-Raman spectrum
- Linewidth of Raman bands
- Low frequency Raman bands
- Low frequency Raman spectrum
- Preresonance Raman spectrum
- Raman intensities

- Raman resonance effect
- Raman second moment
- Rotational fine structure of Raman bands
- Raman

Refractive Index (RI)
The refractive index is the ratio of the velocity of light in a vacuum to its velocity in the substance. The ratio of the sine of the angle of incidence to the sine of the angle of refraction is the index of refraction of the second medium. The refractive index varies with the wavelength of the incident light, temperature and pressure. The values are given at specified temperature and wavelength.

Related Structure (RSTR)
The Related Structure field contains the Accession Numbers (AN's) assigned to substances when a new investigation of the cited compound yields different results, e.g., regarding stereochemistry. The entry contains information about the earlier literature reference and a note as to whether the constitution or configuration assigned to the title compound is wrong or doubtful.

Rotational Spectroscopy (ROT)
The field Rotational Spectrum Description (ROT) contains keywords from a list of controlled terms:

- Microwave spectrum
- Rotational spectrum
- Intensity of microwave bands
- Stark effect
- Rotational-Raman spectrum
- Linewidth of microwave bands
- Intensity of rotational bands
- Linewidth of rotational bands

RX.RAN
The RX.RAN reaction search field contains the reaction accession numbers (RAN).

RX.PAN
The RX.PAN reaction search field contains the product accession numbers (PAN).

Self-Diffusion Coefficient (SDIF)
Self-diffusion is defined as the mutual diffusion caused by a concentration gradient (autodiffusion). The values are given at specified temperatures. You can search for this associated information using the parameter field code /SDIF.T.

Solubility (SLB)
This field describes a multi-component system.
The solubility of one liquid or solid in another is the mass of a substance contained in a solution, which is in equilibrium with an excess of the substance at a specified temperature. You can search for the associated information about the saturation, the temperature, the solvent and the ratio of solvents using the parameter field codes /SLB.SAT, /SLB.T, /SLB.SOL and /SLB.RAT.

Solubility Product (SLBP)
This field describes a multi-component system.
The solubility product is the product of the concentrations of the ions of a substance in a saturated solution of the substance at a specified temperature. You can search for the associated information about the temperature, the solvent and the ratio of solvents using the parameter field codes /SLBP.T, /SLBP.SOL and /SLBP.RAT.

Solution Behavior (SOLM)
This field describes a multi-component system.
The field Solution Behavior Description (/SOLM) contains keywords from the following list of controlled terms:

- Dissolving capacity
- Miscibility
- Solubilizing
- Mutual solubility
- Rate of dissolution
- Solubility [Bunsen absorption coefficient]
- Solubility [Henry constant]
- Solubility [Ostwald absorption coefficient]

Sublimation (SP)
The sublimation point is defined as the temperature at which the vapor pressure above a solid is equal to a specified pressure.

Substance Label (LB)
The Substance Label field describes the location in the patent where a corresponding reference to the substance being searched for can be found.

Surface Tension (ST)
Surface tension is the force per unit length required to create a new unit area of gas-liquid interface. You can search for information about the associated temperature using the parameter field code /ST.T.

Thermal Expansion (TEC)
The thermal expansion coefficient is the ratio of the change in length per unit length or change in volume per unit volume to the change of temperature. The coefficient field is linked to the associated temperature and to the kind of expansion.

Transition Point(s) of Liquid Modification (LPTP)
The temperature at which compounds undergo phase transition in the liquid phase is called the liquid phase transition point. The LPTP field contains the temperature values for the substances.

Transport Data (TRAN)
This field contains information about:
- Thermal conductivity
- Rotational diffusion constant(s)
- Thermal diffusion

Transport Phenomena (TRAM)
This field describes a multi-component system.
The field Transport Phenomena Description (/TRAM) contains keywords from the following list of controlled terms:
- Viscosity
- Diffusion
- Thermal diffusion
- Dynamic viscosity
- Kinematic viscosity
- Bulk viscosity
- Diffusion coefficient
- Binary diffusion coefficient
- Interdiffusion
- Thermal diffusion factor
- Thermal diffusion (Soret coefficient)
- Diffusion thermo effect (Dufour effect)
- Thermal conductivity

Triple Point (TP)
The triple point is the point in a phase diagram where three phases of a substance exist at equilibrium and is fully defined by the temperature and pressure at that point. The Triple Point field contains the temperature values for the substances.

UV/VIS Spectroscopy (UVS)
The field UV Description (UVS) contains keywords from a list of controlled terms:

- Spectrum
- Absorption maxima
- Reflection spectrum
- Singlet-triplet band
- Solvatochromism
- Triplet-triplet band
- Vacuum-UV spectrum
- Absorption spectrum
- Absorption cross-section
- UV excited state absorption
- UV two-photon absorption
- Triplet-singlet absorption spectrum
- Opto-acoustic UV spectrum
- UV/VIS reflection maximum(a)
- X-ray absorption spectrum
- X-ray absorption cross-section
- Band anisotropy
- Oscillator strength
- UV/VIS

Vapor Pressure (VP)
The vapor pressure of a pure liquid or solid is the pressure of the vapor that is in equilibrium with it at a given temperature. You can search for thebassociated temperature using the parameter field code /VP.T.

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