

## Searching Properties in the CAS Registry File

**With the addition of experimental and predicted property data, you can now explore millions of compounds in REGISTRY for molecules with desired properties.**

### Introduction

The CAS Registry File contains both experimentally determined and predicted (calculated) property values. With this information, chemists and informational professionals can explore the compound diversity in REGISTRY for molecules with desired properties.

This STNote has been revised in November 2005; it now includes an overview of searching and displaying property information with search examples.

For additional information on properties in REGISTRY, please refer to:

[www.cas.org/support/stngen/stndoc/properties.html](http://www.cas.org/support/stngen/stndoc/properties.html)

### Searching properties

Each property has its own search field. Most property fields are numeric fields, making it possible for you to search values using numeric operators or ranges or by specifying numeric tolerance. For properties with units, you may specify any units of interest; the default unit is searched whenever a unit is not specified in the query.

Each property name is also posted in the Field Availability (/FA) field. In addition, the records with any property data are posted as PROPERTY DATA/FA.

### Searching property conditions

You may also search the property conditions available for some of the properties. Use the (P) operator to combine the property values with the property conditions.

## Searching LD50 values and conditions

```
=> S 741-745/LD50
L3      11 741 MG/KG - 745 MG/KG /LD50
```

```
=> S L3(P)MOUSE/LD50.ORGAN
      60 MOUSE/LD50.ORGAN
L4      2 L3(P)MOUSE/LD50.ORGAN
```

```
=> D HIT
```

```
L4 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN
```

Median Lethal Dose (LD50)

CODE	VALUE	CONDITION	NOTE
LD50	741 mg/kg	Orgn: mouse Rte: intraperitoneal	(1) CAS

(1) Al'-Assar, F.; Pharmaceutical Chemistry Journal (Translation of Khimiko-Farmatsevticheskii Zhurnal) 2002 V36(11) P598-603 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

```
=> S L3(P)ORAL/LD50.RTE
      19 ORAL/LD50.RTE
L5      8 L3(P)ORAL/LD50.RTE
```

```
=> D HIT
```

```
L5 ANSWER 1 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN
```

Median Lethal Dose (LD50)

CODE	VALUE	CONDITION	NOTE
LD50	>500 mg/kg	Orgn: rat Rte: oral	(1) CAS

(1) Bekhit, Adnan A.; European Journal of Medicinal Chemistry 2003 V38(1) P27-36 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

## Searching property ranges

By default, a numeric property search retrieves property values that are specified as:

- a specific value, e.g., MP=100
- closed range, e.g., MP=90-100 or MP=90±3
- an open-ended range, e.g., MP>100

You may also specify that the retrieved values have to be exact, e.g., MP=100, have to fall within an open-ended range, e.g., MP<90 or MP>100, or have to be in a closed range, e.g., MP=100-120. Use the (P) operator with EXACT/PNT, OPEN RANGE/PNT, or CLOSED RANGE/PNT with the property values to specify the desired type of matching.

For closed range property values, you may also specify the width of the reported range in the Uncertainty Range (/UR) field. Use the (P) operator between a closed range property value and the /UR search term.

For example, searching BP=200(P)UR<=10 retrieves BP values such as 200, 190-200, 200-202, 200-210, 198-204, etc., but would not retrieve the range 200-215 or the open range >200. Exact values are also retrieved because their uncertainty range is 0.

## Searching an exact value for a melting point

```
=> FILE REGISTRY
```

```
=> S 100/MP
```

```
L1          9511 100 DEGC /MP
```

```
=> D L1 HIT
```

```
L1  ANSWER 1 OF 9511  REGISTRY  COPYRIGHT 2004 ACS on  
    STN
```

Melting Point (MP)

CODE	VALUE		NOTE
MP	100-102 deg C	(1)	CAS

(1) Csuk, Rene; Tetrahedron 2003 V59(40) P7887-7895  
CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

```
=> S L1(P)EXACT/PNT
```

```
274480 EXACT/PNT
```

```
L2          1163 L1(P)EXACT/PNT
```

=> D L2 HIT

L2 ANSWER 1 OF 1163 REGISTRY COPYRIGHT 2004 ACS on  
STN

Melting Point (MP)

CODE	VALUE	NOTE
MP	100 deg C	(1) CAS

(1) Sleven, Jurgen; ARKIVOC (Gainesville, FL, United States) 2003(4) P68-82 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

## Displaying properties

Use PRFA (FA) to display the list of property fields available for an answer and their associated codes at no charge.

Use the PROP display format to display all properties for a compound. Use the EPROP format to display only experimental properties. Use the PPROP (CALC) format to display only predicted (calculated) properties.

Experimental property data display in a separate table from the predicted properties, and properties are arranged in alphabetical order by property name. Properties with multiple values are sorted in descending order by the value.

Properties are displayed in a table containing the Field Code, Property Name, Property Value, Conditions (if any), and Note information. Each individual property field is also a display format, e.g., D PKA.

## Displaying available fields

```
=> S 90-92/BP AND 31-33/MP
      22412 90 DEGC - 92 DEGC /BP
      2198 31 DEGC - 33 DEGC /MP
L6      51 90 DEGC - 92 DEGC /BP AND 31 DEGC - 33
        DEGC /MP
```

=> D PRFA 1, 3

L6 ANSWER 1 OF 51 REGISTRY COPYRIGHT 2004 ACS on STN  
Available Properties (PRFA)

CODE	PROPERTY
------	----------

Experimental Data

BP	Boiling Point
MP	Melting Point

L6 ANSWER 3 OF 51 REGISTRY COPYRIGHT 2004 ACS on STN  
Available Properties (PRFA)

CODE | PROPERTY  
=====+

#### Experimental Data

MP Melting Point

#### Calculated Data

BCF Bioconcentration Factor  
BP Boiling Point  
FP Flash Point  
FRB Freely Rotatable Bonds

.  
. .  
. .

### Displaying experimental properties

=> D EPROP 1

L6 ANSWER 1 OF 51 REGISTRY COPYRIGHT 2003 ACS on STN

#### Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Boiling Point (BP)	90-91 deg C	Press: 15 Torr	(1) CAS
Melting Point (MP)	33-37 deg C		(1) CAS

(1) Oohara, Nobuhiko; JP 2003300988 A2 2004 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

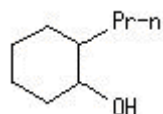
When a property term is searched, HIT or KWIC displays just the row of the table that causes the record to be retrieved and its associated note. QRD (Query Related Display) displays IDE and the row of the table containing the hit property value. If QRD is used for an answer without property information, IDE is displayed.

## Displaying properties with the QRD format

```
=> S 90-92/BP AND 31-33/MP
      22412 90 DEGC - 92 DEGC /BP
      2198 31 DEGC - 33 DEGC /MP
L1      51 90 DEGC - 92 DEGC /BP AND 31 DEGC - 33
      DEGC /MP
```

```
=> D QRD
```

```
L1 ANSWER 1 OF 51 REGISTRY COPYRIGHT 2004 ACS on STN
RN 360787-11-7 REGISTRY
CN Boron, [(1,1-dimethylethyl)methylphosphine]
   trihydro-, (T-4)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN tert-Butylmethylphosphine compd. with borane (1:1)
MF C5 H16 B P
CI CCS
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL
```



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

```
5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)
```

### Experimental Properties

#### Boiling Point (BP)

CODE	VALUE	CONDITION	NOTE
BP	90-91 deg C	Press: 15 Torr	(1) CAS

(1) Oohara, Nobuhiko; JP 2003300988 A2 2004 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

#### Melting Point (MP)

CODE	VALUE	NOTE
MP	33-37 deg C	(1) CAS

(1) Oohara, Nobuhiko; JP 2003300988 A2 2004 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

## Searching and displaying spectra

Spectra information is searched as single words or bound phrases in the /SPEC field. You can display all the spectra using the SPEC display field or specific types of spectra by using other display field codes, e.g., SPEC.IR.

=> FILE REGISTRY

=> S IR/SPEC AND NMR/SPEC

432 IR/SPEC

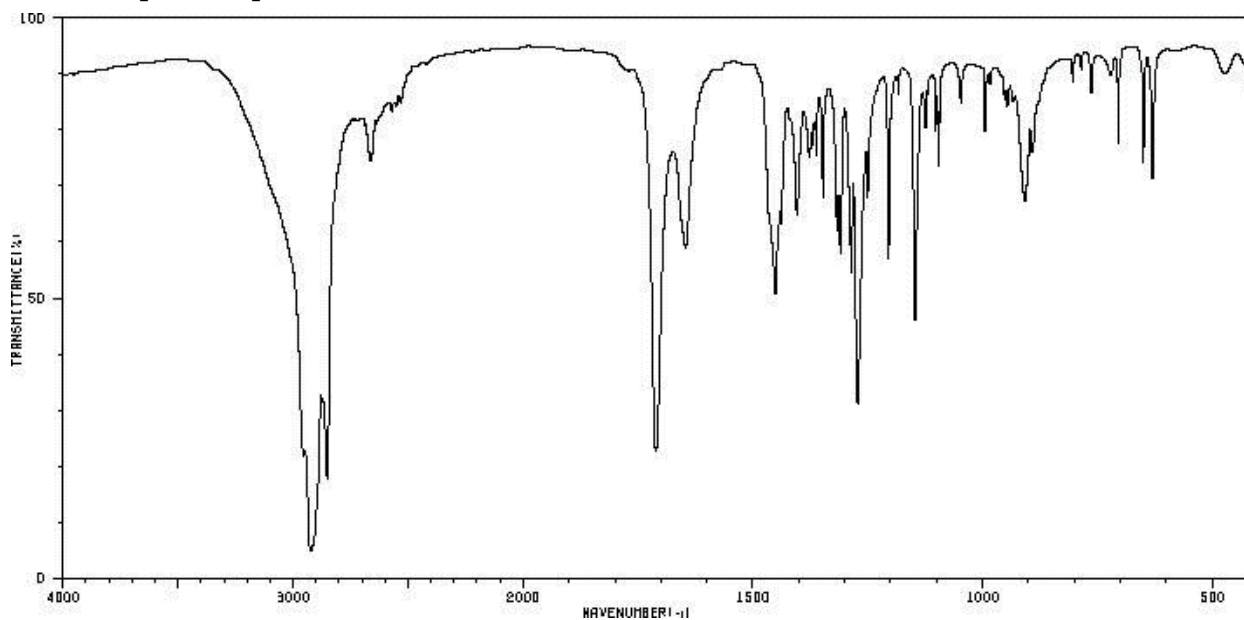
223 NMR/SPEC

L1 188 IR/SPEC AND NMR/SPEC

=> D SPEC

L1 ANSWER 1 OF 188 REGISTRY COPYRIGHT 2005 ACS on STN

IR Absorption Spectra



Spectrum ID:

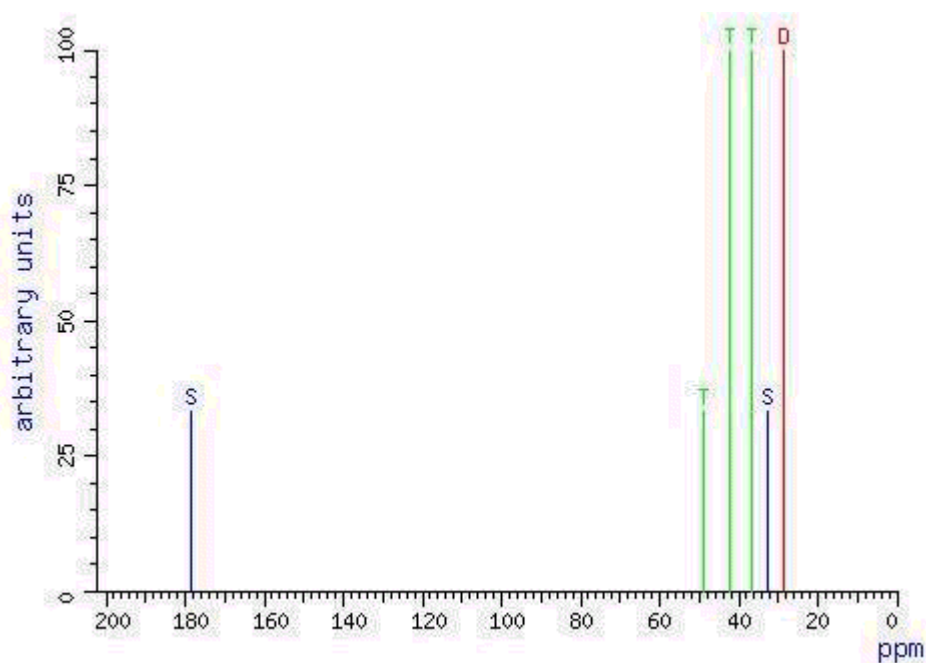
NIDA22444

Source:

"Integrated Spectral Data Base System of Organic Compounds" data are provided by the National Institute of Advanced Industrial Science and Technology (Japan)

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## Carbon-13 NMR Spectra



Spectrum ID: CNCC-57899-233D  
Spectrometer: BRUKER WH-90  
Source: Spectral data are provided by Wiley Subscription Services, Inc. (US)

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## Cost

There is a small charge for displaying all or any combination of property data. Standard search term costs apply. Enter HELP COST at an arrow prompt in REGISTRY or ZREGISTRY for cost information.

## For more information

For more information on searching and displaying property data in REGISTRY, please refer to the REGISTRY and ZREGISTRY Database Summary Sheets at:

[www.cas.org/support/stngen/dbss/index.html](http://www.cas.org/support/stngen/dbss/index.html)

Enter HELP PROPERTIES at an arrow prompt in REGISTRY or ZREGISTRY for information about property data sources and a list of online help messages about searching property data. Enter HELP DIRECTORY at an arrow prompt in each file to see a list of all online help messages for the file.