

Reaxys Proximity Operator

The January 2010 release saw the addition of the PROXIMITY operator - learn here how to best use this option.

Imagine that you need to rapidly find out which N-substituted-fluoroformamide has a boiling point of 20-21°C under a pressure of 25mmHg (25 Torr). How can you do this rapidly? The PROXIMITY operator gives you the solution - you can use this advanced search operator when you need to find correlated properties:

In the Properties (Form-based) tab:

Expand the substance data properties by clicking the '+' sign and then expand the *Physical Data* section. Here enter the required boiling point range value needed and the correlated pressure data. Click on Search to display the found substance.

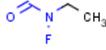
The screenshot shows the Reaxys interface with the 'Substances and Properties' tab selected. In the 'Generate structure from name' section, a chemical structure of N-fluoroformamide is displayed. To the right, there are radio buttons for 'As drawn' (selected) and 'Substructure: on all atoms' (selected). Below these are checkboxes for 'Ignore stereo', 'No salts', 'No mixtures', 'No isotopes', and 'No additional rings', along with a 'Further options' link. A 'Search' button is highlighted with a red box. In the 'Properties (Form-based)' section, the 'Physical Data' section is expanded, showing fields for 'Boiling Point available or = '20-21'' and 'at pressure ='. A red box highlights the 'Search' button.

The core substructure and the required information are highlighted; a click on the black part of the Boiling Point (1 Hit out of 1 view all) hyperlink will display the information and its citation.

[Hit Data](#)
[Boiling Point \(1 Hits out of 1 view all \)](#)

Substances (Grid) Substances (Table) Citations go to Page: Page 1 of 1

Limit to Selection Sort by No of References

Structure	Chemical Name	N° of preparations	Available Data	N° of ref.	Boiling Point
 <input type="checkbox"/> 1 <input type="button" value="Synthesize"/> <input type="button" value="Hide Details"/>	Ethyl-N-fluoroformamid	1 prep out of 2 reactions.	Hit Data (1) Physical Data (2) Spectra (3)	1	20 - 21 °C (25 Torr)

Structure/Compound Data

Reaxys Registry Number: 2425663
CAS Registry Number: 23674-46-6
Chemical Name: Ethyl-N-fluoroformamid
Type of Substance: acyclic

Molecular Formula: C₃H₆FNO
Linear Structure Formula: C₃H₆FNO
Molecular Weight: 91.0851
InChi Key: GSHYENIKGPHZBB-UHFFFAOYSA-N

[Hit Data](#)
[Boiling Point \(1 Hits out of 1 view all \)](#)

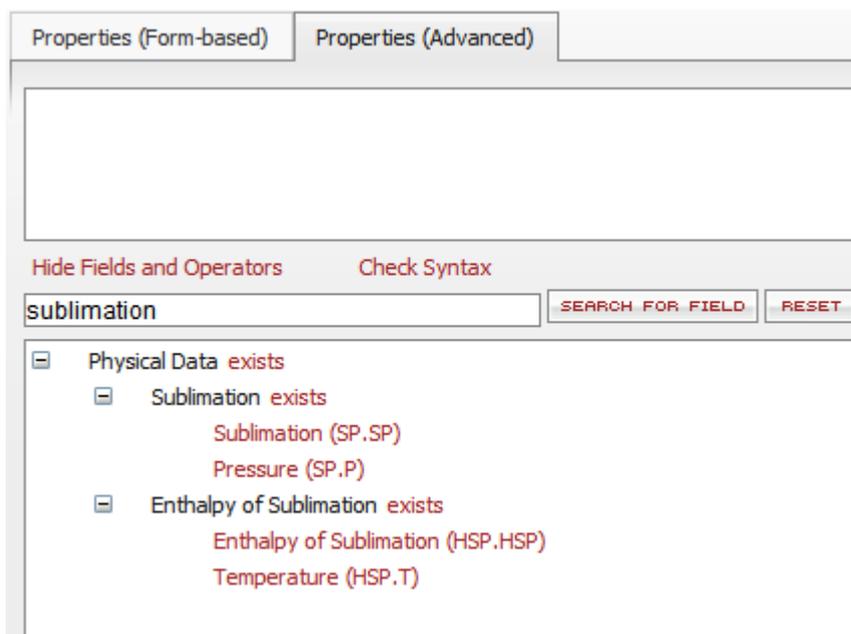
Boiling Point	Pressure	Reference
20 - 21 °C	25Torr	Grakauskas,V.; Baum,K. Journal of Organic Chemistry, 1970 , vol. 35, # 5 p. 1545 - 1549 Full Text View citing articles

Imagine that you now need to purify by sublimation some 2,3-disubstituted-1,4-diazanaphthalene under reduced pressure and you'd like to work at a max temperature of 130°C and under a reduced pressure between 1 and 2 mmHg.

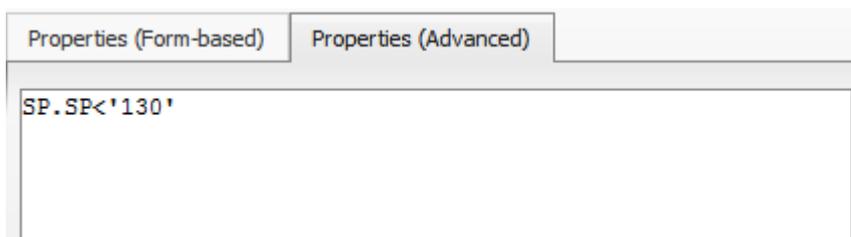
First draw the required scaffold and then check "no additional rings" to avoid any phenazine or other cyclic annelated derivatives that you don't want. To add the sublimation constraint, jump to the Properties (Advanced) tab.

In the Properties (Advanced) tab:

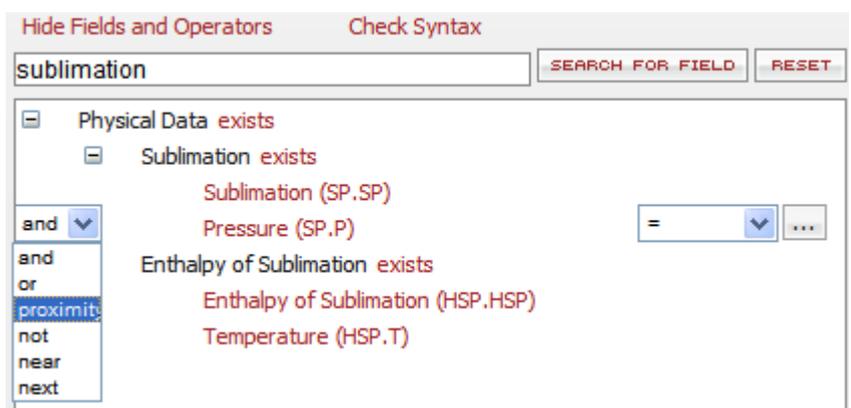
You first need to locate the required field; click on Show Fields and Operators hyperlink and simply type sublimation in the *Search For Field* box and click on the corresponding button to locate the fields. These fields are then immediately displayed:



Click the Sublimation (SP.SP) field, chose '<' as an operator and add the needed value (130). The query is automatically written with the right Syntax in the upper box.



You can now add the correlated constraint - the fact the the sublimation temperature must be linked to a pressure between 1 and 2 Torr. Click the Pressure (SP.P) field and a menu with the possible operators is then displayed. Choose proximity.

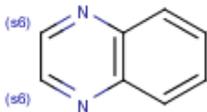


Select '=' as the operator and enter the needed range. The query appears as below:

Reactions Substances and Properties Text, Authors and more

Generate structure from name

Double click this frame and draw structure query



As drawn
Substructure:
on heteroatoms
on all atoms

Ignore stereo
No salts
No mixtures
No isotopes
No additional rings
Further options

Search

Properties (Form-based) Properties (Advanced)

SP.SP<'130' AND SP.P='1 - 2'

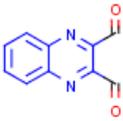
Show Fields and Operators Check Syntax

Clear Query Load Query/Batch Save Query

Advanced Search allows for entering complex property/combination queries following the general rule "<field code> <operator> <field value (s)>".

If you don't know the field code please click the hyperlink **Show Fields and Operators** and select one from the hierarchical tree. If you need additional explanations, please click **here**

Click on Search to display the found results: two substituted quinoxalines are found. For example, the sublimation details for the second hit are as shown below:

	<p>quinoxaline dicarboxyaldehyde-2,3 quinoxaline dicarboxaldehyde-2,3 2,3-diformylquinoxaline quinoxaline-2,3-dicarbaldehyde Chinoxalin-2,3-dicarbaldehyd 2,3-Bis-(formyl)-chinoxalin Chinoxalin-dialdehyd-(2.3)</p>	<p>3 prep out of 11 reactions.</p>	<p>Hit Data (1) Identification Physical Data (7) Spectra (6) Bioactivity/ECotox (1)</p>	<p>12</p>
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Synthesize
Hide Details

Structure/Compound Data

Reaxys Registry Number: 134583
CAS Registry Number: 3138-76-9
Chemical Name: quinoxaline dicarboxyaldehyde-2,3, quinoxaline dicarboxaldehyde-2,3, 2,3-diformylquinoxaline, quinoxaline-2,3-dicarbaldehyde, Chinoxalin-2,3-dicarbaldehyd, 2,3-Bis-(formyl)-chinoxalin, Chinoxalin-dialdehyd-(2.3)
Type of Substance: heterocyclic

Molecular Formula: C₁₀H₆N₂O₂
Linear Structure Formula: C₁₀H₆N₂O₂
Molecular Weight: 186.17

InChi Key: PHWWUGLHWJPYRL-UHFFFAOYSA-N

Hit Data

Sublimation (1 Hits out of 2 view all)

Sublimation	Pressure	Reference
115 - 120 °C	2 Torr	Tetenchuk, K. P.; Dvoryantseva, G. G.; Musatova, I. S.; Elina, A. S. Pharmaceutical Chemistry Journal, 1984, vol. 18, # 5 p. 340 - 345 Title/Abstract Full Text View citing articles

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