

جسجومی ساختار و خواص ترکیبات

www.ShimiPedia.ir

Home - PubMed - NCBI - Windows Internet Explorer

http://www.ncbi.nlm.nih.gov/pubmed/

File Edit View Favorites Tools Help

Home - PubMed - NCBI

NCBI Resources How To Sign in to NCBI

PubMed US National Library of Medicine National Institutes of Health

Search Help

- All Resources
- Chemicals & Bioassays
 - BioSystems
 - PubChem BioAssay
 - PubChem Compound
 - PubChem Structure Search
 - PubChem Substance
 - All Chemicals & Bioassays Resources...
- DNA & RNA
- Data & Software
- Domains & Structures
- Genes & Expression
- Genetics & Medicine
- Genomes & Maps
- Homology
- Literature
- Proteins
- Sequence Analysis
- Taxonomy
- Training & Tutorials
- Variation

Using PubMed

PubMed Quick Links

- Full Text Article
- PubMed FAQs
- PubMed Tutorial
- New and Noteworthy

PubMed Tools

- PubMed Mobile
- Single Citation Matcher
- Batch Citation Matcher
- Clinical Queries
- Topic-Specific Queries

More Resources

- MeSH Database
- Journals in NCBI Databases
- Clinical Trials
- E-Utilities
- LinkOut

more than 22 million citations for biomedical literature from MEDLINE, life science journals, and online books. Citations may include links to full-text content from PubMed Central and publisher web sites.

Home - PubChem Compound - NCBI - Windows Internet Explorer

http://www.ncbi.nlm.nih.gov/pccompound

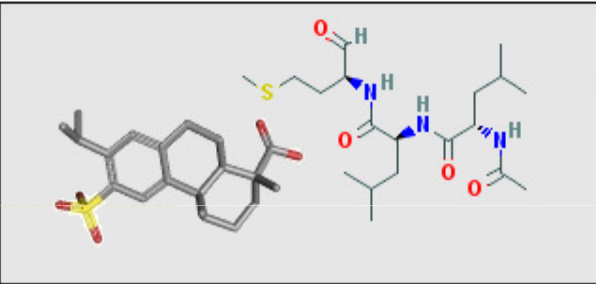
File Edit View Favorites Tools Help

Home - PubChem Compound - NCBI

NCBI Resources How To Sign in to NCBI

PubChem Compound PubChem Compound Search

Limits Advanced Help



PubChem Compound

The PubChem Compound Database contains validated chemical depiction information provided to describe substances in PubChem Substance. Structures stored within PubChem Compounds are pre-clustered and cross-referenced by identity and similarity groups.

Using PubChem

- [Overview](#)
- [PubChem Help](#)
- [PubChem FAQ](#)
- [PubChem Publications](#)
- [PubChem News](#)

PubChem Tools

- [Chemical Structure Search](#)
- [BioActivity Analysis](#)
- [Deposition Gateway](#)
- [Download Facility](#)
- [PubChem FTP](#)

More Resources

- [PubChem Homepage](#)
- [PubChem BioAssay](#)
- [PubChem Substance](#)
- [Structure](#)
- [BioSystems](#)

www.ShimiPedia.ir

Advanced search - PubChem x

www.ncbi.nlm.nih.gov/pcsubstance/advanced

NCBI Resources How To Sign in to NCBI

PubChem Substance Home Help

PubChem Substance Advanced Search Builder

Use the builder below to create your search

[Edit](#) [Clear](#)

Builder

AND

Search

History

There is r

All Fields

HydrogenBondAcceptorCount

HydrogenBondDonorCount

IUPACName

InChI

InChIKey

InactiveAid

InactiveAidCount

IsotopeAtomCount

MeSHDescription

MeSHTerm

MeSHTreeNode

ModifyDate

MolecularWeight

MonoisotopicMass

Patent

PharmAction

PharmActionID

RotatableBondCount

SourceCategory

SourceID

Show index list

Show index list

You are here: NCBI > Chemicals &

GETTING STARTED

- NCBI Education
- NCBI Help Manual
- NCBI Handbook

POPULAR

- PubMed
- Bookshelf
- PubMed Central

FEATURED

- Genetic Testing Registry
- PubMed Health
- GenBank

NCBI INFORMATION

- About NCBI
- Research at NCBI
- NCBI News

Write to the Help Desk

US2010286022A1.pdf

Show all downloads...

www.ShimiPedia.ir

start

Chemistry Databases...

Advanced search - P...

US2010286022A1.pd...

EN

12:26 ب. ق.

Home - PubChem Substance - NCBI - Windows Internet Explorer

http://www.ncbi.nlm.nih.gov/pcsubstance

File Edit View Favorites Tools Help

Home - PubChem Substance - NCBI

NCBI Resources How To Sign in to NCBI

PubChem Substance PubChem Substance Search

Limits Advanced Help



PubChem Substance

The PubChem Substance Database contains descriptions of samples, from a variety of sources, and links to biological screening results that are available in PubChem BioAssay. If the chemical contents of a sample are known, the description includes links to PubChem Compound.

Using PubChem

- [Overview](#)
- [PubChem Help](#)
- [PubChem FAQ](#)
- [PubChem Publications](#)
- [PubChem News](#) 

PubChem Tools

- [Chemical Structure Search](#)
- [BioActivity Analysis](#)
- [Deposition Gateway](#)
- [Download Facility](#)
- [PubChem FTP](#)

More Resources

- [PubChem Homepage](#)
- [PubChem BioAssay](#)
- [PubChem Compound](#)
- [Structure](#)
- [BioSystems](#)

www.ShimiPedia.ir

PubChem Structure Search - Windows Internet Explorer

http://pubchem.ncbi.nlm.nih.gov/search/#

File Edit View Favorites Tools Help

PubChem Structure Search


NCBI

PubChem Structure Search


PubChem Compound Search

Limits Advanced search Help


Search By: Name/Text Identity/Similarity **Substructure/Superstructure** Molecular Formula 3D Conformer Saved Search

 Draw a Structure CID, SMILES/SMARTS, InChI Structure File

the PubChem editor to make a structure

 Options

Substructure

 Filters

www.ShimiPedia.ir

Broadband SMILES C1(=CC=C(C=C1)C(C)N)C(=O)[H]

New Undo Clear Style Delete Query

Line styles: single, double, triple, arrow, dashed, wavy, zigzag, S/A, D/A, S/D

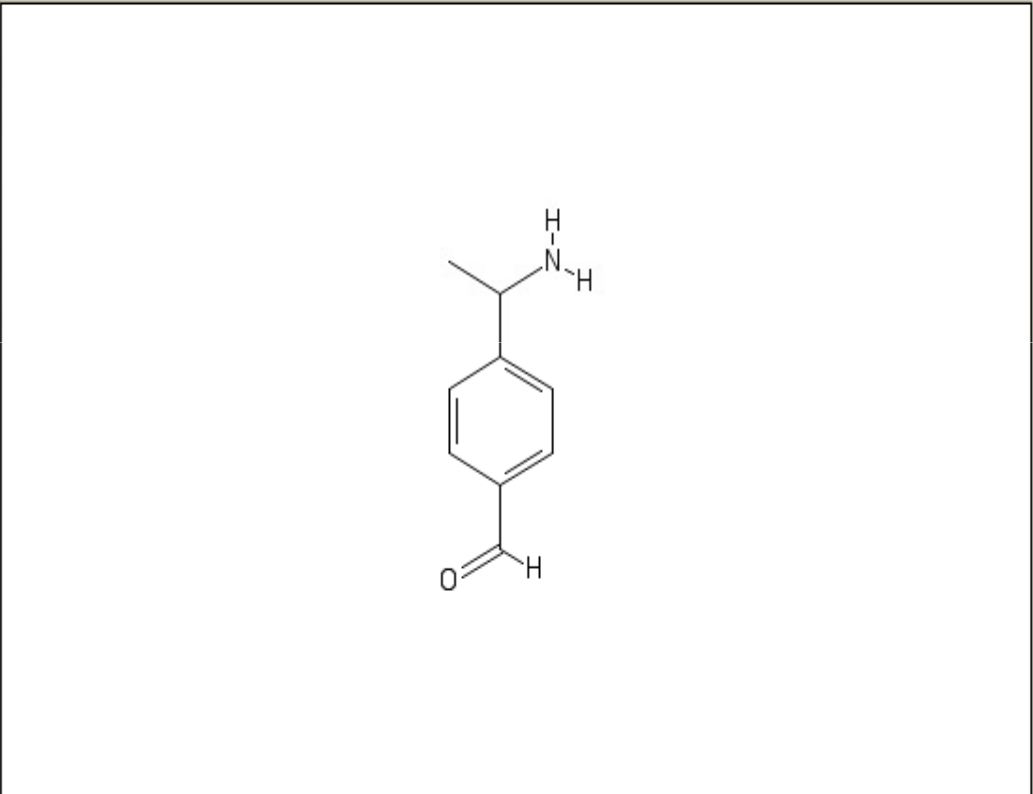
Shapes: triangle, square, pentagon, hexagon, heptagon, octagon, benzene ring, grid, plus, minus, CHO, CO₂H, NO₂, SO₃H

H		?	?						He
Li	Be			B	C	N	O	F	Ne
Na	Mg			Al	Si	P	S	Cl	Ar
K	Ca	Sc	Sc	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Y	In	Sn	Sb	Te	I	Xe
Cs	Ba	Lu	Lu	Tl	Pb	Bi	Po	At	Rn

Export MDL Molfile Done

Hydrogen Keep AsIs Help

Import Browse...



PubChem Structure Search - Windows Internet Explorer

http://pubchem.ncbi.nlm.nih.gov/search/#

File Edit View Favorites Tools Help

PubChem Structure Search

NCBI


PubChem Structure Search

PubChem Compound Search

Limits Advanced search Help

Search By: Name/Text Identity/Similarity **Substructure/Superstructure** Molecular Formula 3D Conformer Saved Search

Draw a Structure CID, SMILES/SMARTS, InChI Structure File

 Edit Search

Options

Substructure

Filters

www.ShimiPedia.ir

Internet 100%

start Chemical inform... Chemical Inform... PubChem Struct... aminoethylphos... Microsoft Power... EN 05:28

Display Settings: Summary, 20 per page, Sorted by Default order Send to: Filters: Manage Filters

Results: 1 to 20 of 579 << First < Prev Page 1 of 29 Next > Last >>

- 1.  [Forphenicine: 4-Formyl-3-hydroxyphenylglycine; BRN 5008292 ...](#)
MW: 195.172060 g/mol MF: C₉H₉NO₄
IUPAC name: 2-amino-2-(4-formyl-3-hydroxyphenyl)acetic acid
CID: 42560
[Summary](#) [Similar Compounds](#) [PubMed \(MeSH Keyword\)](#)
- 2.  [NSC683400: AC1L8VY7; NSC-683400 ...](#)
MW: 519.631880 g/mol MF: C₃₀H₃₇N₃O₅
IUPAC name: [2-(cyclohexylcarbamoxyloxymethyl)-7-formyl-1-methylbenzo[g]i...
CID: 388464
[Summary](#) [Similar Compounds](#) [Tested in 62 BioAssays](#)
- 3.  [4-imidazo\[2,1-b\]\[1,3\]thiazol-6-ylbenzaldehyde; AQ-776/42801094; NSC707998 ...](#)
MW: 228.269720 g/mol MF: C₁₂H₉N₂O₅
IUPAC name: 4-imidazo[2,1-b][1,3]thiazol-6-ylbenzaldehyde
CID: 398284
[Summary](#) [Similar Compounds](#)
- [AQ-776/42801253; NSC708001; AC1L9GA9 ...](#)

Actions on your results

-  **BioActivity Analysis**
Analyze the BioActivities of the compounds
-  **Structure Clustering**
Cluster structures based on structural similarity
-  **Structure Download**
Download the structures in various formats

Refine your results

- Chemical Properties**
Rule of 5 (465)
- BioActivity Experiments**
BioAssays, Active (6) 
BioAssays, Tested (14) 
- Depositor Category**
Biological Properties (247)
Chemical Vendors (84)
Journal Publishers (121)

Search and share chemistry

Simple Structure Advanced History

Search ChemSpider

Matches any text strings used to describe a molecule.



Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID ?

What is ChemSpider?

ChemSpider is a free chemical structure database providing fast text and structure search access to over 35 million structures from hundreds of data sources.

Search by chemical names

- Systematic names
- Synonyms
- Trade names
- Database identifiers

Search by chemical structure

- Create structure-based queries
- Draw structures in the web page
- Use structure files from your computer

Find important data

- Literature references
- Physical properties
- Interactive spectra
- Chemical suppliers

Advertisements

See More Differences that Matter

Take your metabolomics and lipidomics research to the next level

Learn More

Thermo SCIENTIFIC

ANSWER MORE QUESTIONS

THE NEW AGILENT 6545 Q-TOF LC/MS

LEARN MORE

Agilent

Give Feedback

Generate Leads

Blog

Subscribe

[Introduction to the new ChemSpider website](#)

[What's new with ChemSpider?](#)

35 Million
chemical structures

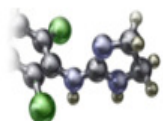
Yahoo! Mail: The best web-based email!
https://login.yahoo.com/config/login_verify2?intl=us&lang=en-US&src=ym



TOXNET TOXICOLOGY DATA NETWORK

[Help](#) | [FAQs](#) | [TOXNET Fact Sheet](#) | [Training Manual & Schedule](#)

[TOXNET Home](#) > [ChemIDplus Advanced](#)



ChemIDplus
A TOXNET DATABASE
[Lite](#) • [Browse](#) • [Advanced](#)

[Search](#) [Clear](#) [History](#) [Help](#)

Substance Identification *i*

(automatic) (automatic)

Data is available for 409,050 records.

Toxicity *i*

Test: (any) between (mg/kg or ppm)

Species: (any)

Route: (any)

Effect: (any)

Toxicity data is available for 139,289 records.

Physical Properties *i*

Melting Point

between

Either Measurement Type

Physical property data is available for 25,442 records and was provided by [Syracuse Research Corporation](#).

Structure *i*

[Draw](#)

Powered by [ChemAxon Marvin](#)

Use: Marvin for JavaScript

[Import MOL](#)

Structure Search Options *i*

- Substructure Search
- Similarity Search 80 %
- Exact (parent only)
- Flex (parent, salts, mixture)
- Flexplus (parent, all variations)

Structure data is available for 320,207 records.

Molecular Weight *i*

between

Molecular weight data is available for 320,207 records.

eMolecules

Products ▾ About Us ▾ My Account ▾ Shopping Cart Support ▾

Quick Links

Current Suppliers
[Building Blocks](#)
[Screening Compounds](#)

Supplier Links

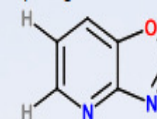
[Supplier Benefits](#)
[Submit your Catalog](#)

[Need help Ordering?](#)
[Give us your feedback](#)

I want to buy: [What's this?](#)

Did You Know

You can block substituents at a particular position by drawing explicit hydrogen atoms.



[next hint...](#)

Search Named Chemicals

Name: [Lipitor](#), [Ibuprofen](#) CAS Num: [15687-27-1](#) SMILES: [S=C=NC](#)

SciFinder - Sign In - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Refresh Print Stop

Address <https://scifinder.cas.org/scifinder/login.jsf?TYPE=33554433&REALMOID=06-b7b15cf0-642b-1005-963a-830c809fff21&GUID=&SMAUTHREASON=0&METHOD=GET&SMAGENTNAME> Go

SciFinder® ...Part of the process™

Sign In

Username

Password

Remember my username

[Forgot Username or Password?](#)

Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.

Welcome to SciFinder!

Friendly Competition . . .

SciFinder has all the substance, chemistry, and related scientific information you will need to develop innovative ideas that will outsmart the competition. So, log in now and find your inspiration.

The new CAS Chemistry Research Report: Human Genome Discoveries Spur Growth of Cancer Treatments focuses on fifty years of journal and patent publications in the CAS databases and how Gleevec changed cancer therapy and personalized medicine.

CAS Database Update

Digital Object Identifiers (DOIs) are becoming a standard for online document identification. SciFinder now offers access to more than 8 million validated DOIs in the CAplus database. Within SciFinder, you can search by and display DOIs, as well as include them in reference material exported to bibliographic management packages. Many more DOIs will be added to CAplus and available through SciFinder by the end of 2010.

New SciFinder Features Increase Research Productivity and Expand Access to Substance-Related Patent

What is SciFinder?

SciFinder is a research discovery tool that allows you to explore the CAS databases containing literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!

[About SciFinder](#) | [SciFinder Support and Training](#) | [CAS Databases](#)

Done Internet

www.ShimiPedia.ir

SciFinder در پایگاه اطلاعاتی Chemical Abstract جستجو کرده و در مورد فرمول مولکولی، نام شیمیائی، ساختار مولکولی، ساختار واکنش ها، نام مؤلف یا عناوین شیمیائی اطلاعات جامعی فراهم می سازد.

The screenshot displays the SciFinder web interface. At the top, there are navigation tabs for 'References', 'Substances', and 'Reactions'. A user is logged in as 'Yifat Belous' with a 'Sign Out' option. The main section is titled 'Explore References' and features a search bar with a 'Search' button. Below the search bar, there are several filter categories:

- Research Topic:** A dropdown menu with options: Author Name, Company Name, Document Identifier, Journal, Patent, and Tags.
- Publication Year(s):** A text input field with examples: 1995, 1995-1999, 1995-, -1995.
- Document Type(s):** A grid of checkboxes for various document types: Biography, Book, Clinical Trial, Commentary, Conference, Dissertation, Editorial, Historical, Journal, Letter, Patent, Preprint, Report, and Review.
- Language(s):** A grid of checkboxes for various languages: Chinese, English, French, German, Italian, Japanese, Polish, Russian, and Spanish.

On the right side of the interface, there are three panels:

- Saved Answer Sets:** Shows a set named 'minsky' with a 'View All' link and an 'Import' button.
- Keep Me Posted Results:** States 'No profiles exist'.
- My Connections:** States 'No invitations to connect', 'No outstanding sent invitations', and 'No connection with colleagues'.

A watermark 'www.ShimiPedia.ir' is visible across the bottom of the page. The browser's taskbar at the bottom right shows the Hebrew word 'הסתיים' (Completed).

SciFinder - Explore References - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Refresh Print View Home

Address <https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf> Go

SciFinder®

Welcome Yifat Belous | Sign Out

Explore References Explore Substances Explore Reactions

Saved Answer Sets Help
Keep Me Posted Results History
My Connections Preference

Explore References

Research Topic Search

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds

Author Name
Company Name
Document Identifier
Journal
Patent
Tags

Publication Year(s)
Examples: 1995, 1995-1999, 1995-, -1995

Document Type(s)

<input type="checkbox"/> Biography	<input type="checkbox"/> Dissertation	<input type="checkbox"/> Patent
<input type="checkbox"/> Book	<input type="checkbox"/> Editorial	<input type="checkbox"/> Preprint
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Historical	
<input type="checkbox"/> Commentary	<input type="checkbox"/> Journal	
<input type="checkbox"/> Conference	<input type="checkbox"/> Letter	

Language(s)

<input type="checkbox"/> Chinese	<input type="checkbox"/> German
<input type="checkbox"/> English	<input type="checkbox"/> Italian

Saved Answer Sets ⓘ
No answer sets

Keep Me Posted Results ⓘ
No profiles exist

My Connections ⓘ
No invitations to connect
No outstanding sent invitations
No connection with colleagues

www.ShimiPedia.ir

Done Internet

گزینه های اصلی جستجو شامل جستجوی مقالات از طریق اطلاعات کتابشناسی یا ترکیبات شیمیایی یا واکنش های شیمیایی است.

SciFinder - Explore References - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Refresh Home Search Favorites Print Mail Stop

Address: https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf Go

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Yifat Belous | Sign Out

Saved Answer Sets Help
Keep Me Posted Results History
My Connections Preference

Explore References

Research Topic Search

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds

Research Topic

- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

Publication Year(s)

Examples: 1995, 1995-1999, 1995-, -1995

Document Type(s)

<input type="checkbox"/> Biography	<input type="checkbox"/> Dissertation	<input type="checkbox"/> Patent
<input type="checkbox"/> Book	<input type="checkbox"/> Editorial	<input type="checkbox"/> Preprint
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Historical	<input type="checkbox"/> Report
<input type="checkbox"/> Commentary	<input type="checkbox"/> Journal	<input type="checkbox"/> Review
<input type="checkbox"/> Conference	<input type="checkbox"/> Letter	

German Polish
 Italian Russian

Saved Answer Sets ⓘ
No answer sets
Import

Keep Me Posted Results ⓘ
No profiles exist

My Connections ⓘ
No invitations to connect
No outstanding sent invitations
No connection with colleagues

Done Internet

جستجوی کتابشناسی با گزینه های متفاوتی امکان پذیر است.

www.ShimiPedia.ir



Explore References Explore Substances Explore Reactions

Saved Answer Sets Help
Keep Me Posted Results History
My Connections Preference

Welcome Yifat Belous | Sign Out

Create Keep Me Posted "Research Topic "nanofabrication" with limiters > references (2959)

Explore References

Research Topic

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds

Author Name
 Company Name
 Document Identifier
 Journal
 Patent
 Tags

Publication Year(s)

Examples: 1995, 1995-1999, 1995-, -1995

Document Type(s)

<input type="checkbox"/> Biography	<input type="checkbox"/> Dissertation	<input checked="" type="checkbox"/> Patent
<input type="checkbox"/> Book	<input type="checkbox"/> Editorial	<input checked="" type="checkbox"/> Preprint
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Historical	<input type="checkbox"/> Report
<input type="checkbox"/> Commentary	<input checked="" type="checkbox"/> Journal	<input type="checkbox"/> Review
<input type="checkbox"/> Conference	<input type="checkbox"/> Letter	

Language(s) Chinese German Polish

Saved Answer Sets

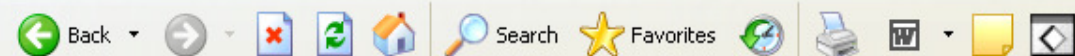
No answer sets

Keep Me Posted Results

No profiles exist

My Connections

No invitations to connect
 No outstanding sent invitations
 No connection with colleagues



Saved Answer Sets | Help
Keep Me Posted Results | History
My Connections | Preferences

Welcome Yifat Belous | Sign Out

Create Keep Me Posted Research Topic "transition temperature of Poly..." with limiters

Research Topic Candidates

5 Topics 0 Selected

[Select All](#) [Deselect All](#)

Research Topic Candidates

References

- | | | |
|--------------------------|---|-------|
| <input type="checkbox"/> | 34 references were found containing "transition temperature of Polystyrene" as entered. | 34 |
| <input type="checkbox"/> | 800 references were found containing the two concepts "transition temperature" and "Polystyrene" closely associated with one another. | 800 |
| <input type="checkbox"/> | 2105 references were found where the two concepts "transition temperature" and "Polystyrene" were present anywhere in the reference. | 2105 |
| <input type="checkbox"/> | 79951 references were found containing the concept "transition temperature". | 79951 |
| <input type="checkbox"/> | 46567 references were found containing the concept "Polystyrene". | 46567 |

[Get References](#)

SciFinder - Reference Answer Set - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Refresh Print W Stop Home

Address: https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf Go

References **Get Substances** **Get Reactions** **Get Cited** **Get Citing** **Get Full Text** **Combine Answer Sets**

800 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 40 Display: [List Icon]

1. **High molecular weight polystyrene-nylon graft copolymers with novel controlled architectures**
 By Ilinca, S. J.; Duchateau, R.; Koning, C. E.
 From Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (2009), 50(2), 202-203. Language: English, Database: CAPLUS
 Atom transfer radical polymn. (ATRP) and reactive extrusion were applied for the successful synthesis of novel graft copolymers **polystyrene-g-polyamide-6** (6) with a controlled length and no. of brushes at the chain ends. The whole process consists of three stages: (i) prepn. by ATRP of α,ω -dibromo telechelic **polystyrene** (1) with various masses between 2 kg/mol and 100 kg/mol, (ii) use of (1) as macroinitiator for ATRP of styrene (2) and maleimide (3), furnishing [(styrene/maleimide)-**polystyrene**-(styrene/maleimide)] (SMI-b-PS-b-SMI) triblock copolymers (4) with maleimide contents up to 20 wt% ...
 Substances Reactions Citing Full Text Link 0 Comments 0 Tags

2. **Radical polymerization of styrene dimer and radical copolymerization of styrene dimer with styrene**
 By Ohara, Masayuki; Hashimoto, Tamotsu; Urushisaki, Michio; Sakaguchi, Toshikazu; Sawaguchi, Takashi; Sasaki, Daisuke
 From Kobunshi Ronbunshu (2009), 66(11), 498-502. Language: Japanese, Database: CAPLUS
 Radical polymns. of a styrene dimer (SD), 2,4-diphenyl-1-butene, and thermal degrdn. product of **polystyrene** for chem. recycling, were investigated under variable reaction conditions. BPO-initiated radical polymn., atom transfer radical polymn. (ATRP), stable free radical polymn. (SFRP), and reversible addn.-fragmentation chain transfer (RAFT) polymn. conditions. The homopolymns. of SD proceeded probably because of steric hindrance of bulky α -substituent of SD. Radical copolymns. of SD with styrene and relatively high-mol.-wt.-copolymers [the no.-av.-mol.- wts....
 Substances Reactions Citing Full Text Link 0 Comments 0 Tags

3. **Cationic polymerization of styrene dimer and styrene trimer as thermal degradation products of polystyrene**
 By Ohara, Masayuki; Hashimoto, Tamotsu; Urushisaki, Michio; Sakaguchi, Toshikazu; Sawaguchi, Takashi; Sasaki, Daisuke
 From Kobunshi Ronbunshu (2009), 66(11), 483-490. Language: Japanese, Database: CAPLUS
 Cationic polymns. of a styrene dimer (SD), 2,4-diphenyl-1-butene, and a styrene trimer (ST) and hexene, as thermal degrdn. products of **polystyrene** were carried out with the HCl/SnCl₄ and SnCl₄/SnCl₄-initiating systems. The polymns. reached 100% monomer conversion and the no.-av. mol. wt. of the products were about 400-600. The structure of the products was analyzed by GC-MS, FAB-MS, and ¹³C NMR spectroscopy. These spectroscopic results showed that the main products from SD and ST were linear olefinic

Analysis Refine

Analyze by: Author Name

Click bar to view only those references within the current answer set

Torkelson John M	20
Simon Sindee L	12
Roth Connie B	10
Jean Y C	9
Fukao Koji	8
Kim Jin Kon	8
Lee L James	8
Ugur Saziye	8
Chen Hongmin	7

More detailed analysis based on CAS

Done Internet

با انتخاب گزینه مناسب تمام اطلاعات مورد نظر از مقاله استخراج و نمایش داده می شود.

SciFinder - Substance Answer Set - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Search Favorites

Address: <https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf> Go

1. Substance Detail
9011-14-7

80-62-6
C₅H₈O₂

CC(=O)C(=O)OC

(C₅H₈O₂)_x

2-Propenoic acid, 2-methyl-, methyl ester, homopolymer

~85,621 References

Reactions

Commercial Sources

Regulatory Information

Link

2. Substance Detail
9003-53-6

100-42-5
C₈H₈

C=Cc1ccccc1

(C₈H₈)_x

Benzene, ethenyl-, homopolymer

~140,325 References

Reactions

Commercial Sources

Regulatory Information

Link

3. Substance Detail
124-38-9

O=C=O

C O₂

Carbon dioxide

~263,773 References

Reactions

Commercial Sources

Regulatory Information

Link

answer set

Commercially Available 4

Show More

4. Substance Detail
67-64-1

CC(=O)C

www.ShimiPedia.ir

درمورد هر ترکیب اطلاعات اضافی هم ارائه می شود.

Internet

SciFinder - Explore Substances - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Refresh Print Mail Stop

Address <https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf> Go

SciFinder® Explore References **Explore Substances** Explore Reactions

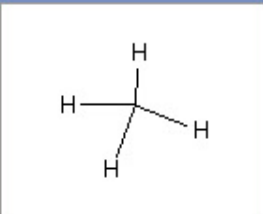
Welcome Yifat Belous | Sign Out

Create Keep Me Posted "Substance Identifier "83-67-0" > substances (1)

Explore Substances

Chemical Structure **Chemical Structure**

Molecular Formula
Substance Identifier



Click image to change structure or view detail

Search type: Exact Structure
 Substructure
 Similarity

Show precision analysis

Characteristic(s)

- Single component
- Commercially available
- Included in reference(s)

Class(es)

- Alloys
- Coordination compounds
- Polymers

Saved Answer Sets No answer sets

Keep Me Posted Results No profiles exist

My Connections No invitations to connect
No outstanding sent invitations
No connection with colleagues

www.ShimiPedia.ir

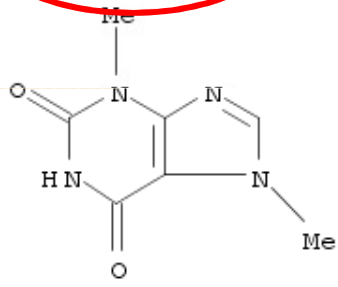
Internet

با رسم ساختار یا ارسال فایل آن می توان
اطلاعات مورد نیاز را بدست آورد.

Substances [Get References](#) [Get Reactions](#) [Get Commercial Sources](#) [Combine Answer Sets](#)

1 Substance 0 Selected Keep Selected Remove Selected Save Print Export
Select All Deselect All Sort by: CAS Registry Number Answers per Page [15]
View: [Icons]

1. Substance Detail
83-67-0



C₇ H₈ N₄ O₂
1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-
[~3,630 References](#)
[Reactions](#)
[Commercial Sources](#)
[Regulatory Information](#)
[Link](#)

Analysis Refine
Analyze by: [Commercial Availability](#)
Click bar to view only those substances within the current answer set
Commercially Available 1
[Show More](#)

Predicted Properties: [Biological](#) [Chemical](#) [Density](#) [Lipinski and Related](#) [Spectra](#) [Structure-related](#)

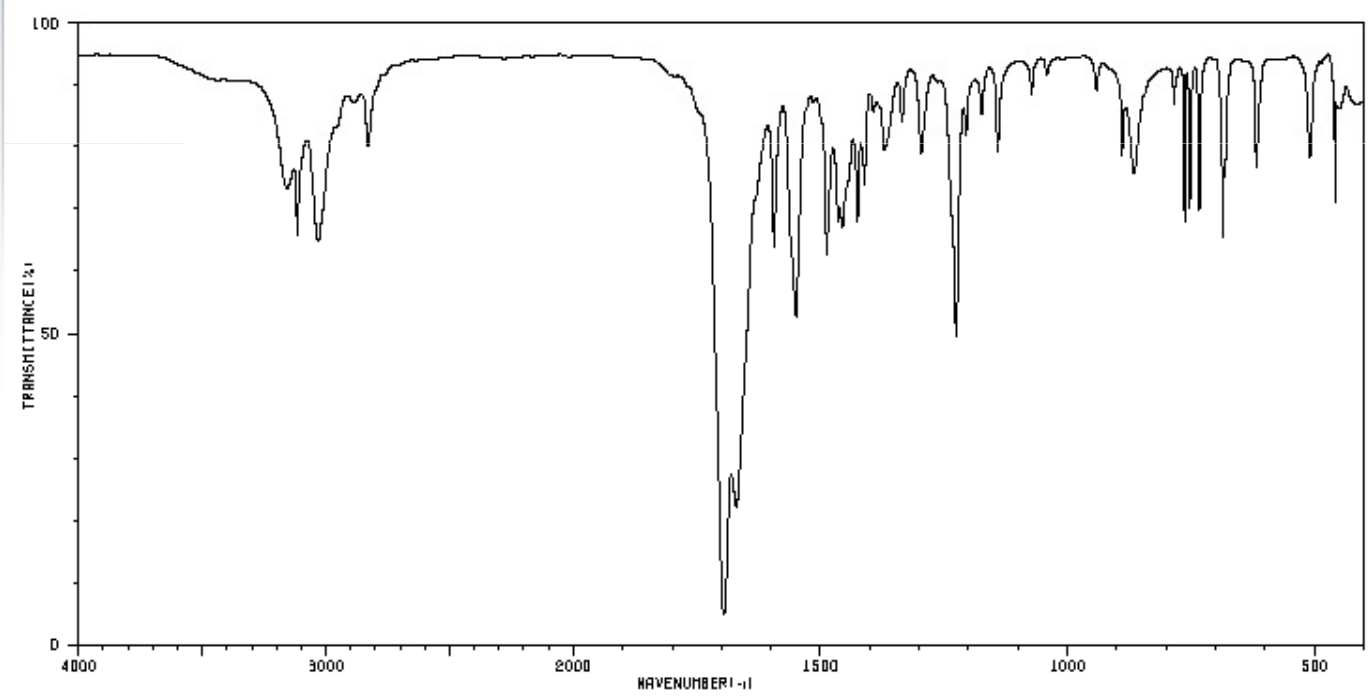
Biological Properties	Value	Condition	Note	Top
Bioconcentration Factor	1.0	pH 1 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 2 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 3 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 4 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 5 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 6 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 7 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 8 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 9 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 10 Temp: 25 °C	(55)	

Chemical Properties	Value	Condition	Note	Top
Koc	6.99	pH 1 Temp: 25 °C	(55)	
Koc	9.31	pH 2 Temp: 25 °C	(55)	
Koc	9.63	pH 3 Temp: 25 °C	(55)	
Koc	9.66	pH 4 Temp: 25 °C	(55)	
Koc	9.66	pH 5 Temp: 25 °C	(55)	
Koc	9.66	pH 6 Temp: 25 °C	(55)	
Koc	9.65	pH 7 Temp: 25 °C	(55)	
Koc	9.54	pH 8 Temp: 25 °C	(55)	
Koc	8.59	pH 9 Temp: 25 °C	(55)	
Koc	4.33	pH 10 Temp: 25 °C	(55)	
logD	-0.86	pH 1 Temp: 25 °C	(55)	
logD	-0.74	pH 2 Temp: 25 °C	(55)	
logD	-0.72	pH 3 Temp: 25 °C	(55)	
logD	-0.72	pH 4 Temp: 25 °C	(55)	
logD	-0.72	pH 5 Temp: 25 °C	(55)	

Create Keep Me Posted Substance Identifier "83-67-0" > substances (1) > 83-67-0 > IR Absorption Spectrum (NIDA63087)

IR Absorption Spectrum

Print



Spectrum ID

NIDA63087

Spectrometer

Nicolet 170SX or JASCO FT/IR-410

Source


Integrated Spectral Database System of Organic Compounds. (Data were obtained from the National Institute of Advanced Industrial Science and Technology (Japan))

Reaxys - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Refresh Home Search Favorites Print Mail Stop

Address <https://www.reaxys.com/reaxys/secured/start.do;jsessionid=122384136E5DD914024B1CFDAA86E531> Go

 **reaxys**[®]

Anonymous user (132.77.4.43)

Query Results Synthesis Plans History My Alerts My Settings Help Register Login

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

COPY TO REACTIONS TAB CLEAR

Properties (Form-based) Properties (Advanced) Search

Substance Data
 Bibliographic Data

Clear Query Load Query/Batch Save Query

www.ShimiPedia.ir

Done Internet

Reaxys - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Refresh Home Search Favorites Print Mail Stop

Address <https://www.reaxys.com/reaxys/secured/start.do;jsessionid=122384136E5DD914024B1CFDAA86E531> Go


reaxys Anonymous user (132.77.4.43)

Query Results Synthesis Plans History My Alerts My Settings Help Register Login

Reactions Substances and Properties Text, Authors and more

Generate structure from name

Double click this frame and draw structure query



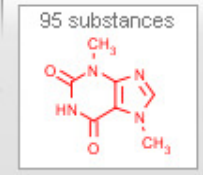
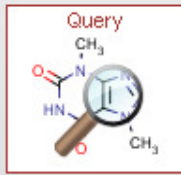
As drawn
 Substructure:
 on heteroatoms
 on all atoms

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

Properties (Form-based) Properties (Advanced)

Substance Data
 Bibliographic Data

Done Internet



Create Alert

95 substances out of 545 citations

- Filter by:
- Sub-structure
 - Molecular Weight
 - Number of Fragments
 - Physical Data
 - Spectroscopic Data
 - Bioactivity
 - Natural Product
 - Document Type
 - Authors
 - Patent Assignee
 - Journal Title
 - Publication Year

Substances (Grid) Substances (Table) Citations go to Page Page 1 of 11

Limit to Output Print Zoom in Zoom out Hide Sort by No of References

Structure	Chemical Name	N° of preparations All Preps All Reactions	Available Data	N° of ref.	Boiling Point
<input type="checkbox"/> 1 Synthesize Show Details	3,7-dimethyl xanthine theobromine 3,7-dimethylxanthine 3,7-dimethylxantine paraxanthine Theobromine 3,7-dimethyl-3,7-dihydro-purine-2,6-dione	58 prep out of 368 reactions.	Identification Physical Data (167) Spectra (75) Bioactivity/Ecotox (91) Use/Application (218) Natural Product (19)	501	
<input type="checkbox"/> 2 Show Details	3,7-dimethyl-3,7-dihydro-purine-2,6-dione, theobromine; salicylate 3,7-dimethyl-3,7-dihydro-purine-2,6-dione; salicylate (1:1) 3,7-Dimethyl-3,7-dihydro-purin-2,6-dion, Theobromin; Salicylat 3,7-Dimethyl-3,7-dihydro-purin-2,6-dion; Salicylat (1:1)	0 prep out of 1 reactions.	Physical Data (1) Spectra (1)	3	

www.ShimiPedia.ir