



**CHEMICAL ABSTRACTS SERVICE: THE GOLD STANDARD FOR CHEMICAL
SUBSTANCE INFORMATION**

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ABSTRACT

A chemical is a form of matter that has constant chemical composition and characteristic properties. It cannot be separated into components by physical separation methods, i.e., without breaking chemical bonds. Chemical substances can be chemical elements, chemical compounds, ions or alloys. Evan Jay Crane (February 14, 1889 – December 30, 1966) was an American chemist and the editor of Chemical Abstracts 1915-1958. Chemical Abstracts say about the detail history of chemical compound either organic or inorganic.

KEYWORDS: CAS REGISTRYSM, CHEMINDEX, CAS Registry Numbers, CAPLUS, CASSI, CASREACT[®], CHEMCATS[®], CHEMLIST[®], CIN[®], MARPAT[®], Organic compounds, Inorganic compounds, Metals Alloys, Minerals, Coordination compounds, Organometallics, Elements, Isotopes, Nuclear particles, Proteins and nucleic acids, Polymers, Nonstructurable materials (UVCBs).

INTRODUCTION

Chemical Abstracts Service (CAS) is a division of the American Chemical Society. It is a source of chemical

information. CAS is located in Columbus, Ohio, United States.



Figure 1: American Chemical Society building A for Chemical Abstract Headquarter, Ohio.

Formation: 1907, Headquarters: Columbus, Ohio,
Location: United States, Official language: English,
President: Manuel Guzman, Website:
<http://www.cas.org/>

Chemical Abstracts is a periodical index that provides summaries and indexes of disclosures in recently published scientific documents. Approximately 8,000

journals, technical reports, dissertations, conference proceedings and new books, in any of 50 languages, are monitored yearly, as are patent specifications from 27 countries and two international organizations. Chemical Abstracts ceased print publication on January 1, 2010.

History

Chemical Abstracts (CA) began as a volunteer effort and developed from there. The use of volunteer abstractors was phased out in 1994. Chemical Abstracts has been associated with the American Chemical Society in one way or another since 1907.^[1]

Mailing address: Chemical Abstracts Service, P.O. Box 3012, Columbus, Ohio 43210, U.S.A. Street address: Chemical Abstracts Service, 2540 Olentangy River Road, Columbus, OH 43202, U.S.A. Phone: 800-848-6538 (North America), 614-447-3600 (worldwide), Fax: 614-447-3713, E-mail: help@cas.org

For many years, beginning in 1909, the offices of Chemical Abstracts were housed in various places on the campus of Ohio State University in Columbus, Ohio. In 1965, CAS moved to a new 50-acre (200,000m²) site on the west bank of the Olentangy River, just north of the Ohio State campus. This campus became well known in the Columbus area and famous as the site of many Columbus Symphony Orchestra pop concerts. In 2009, the campus consisted of three buildings.

1. In 1907, William A. Noyes had enlarged the Review of American Chemical Research, an abstracting publication begun by Arthur Noyes in 1895 that was the forerunner of Chemical Abstracts. When it became evident that a separate publication containing these abstracts was needed, Noyes became the first editor of the new publication, Chemical Abstracts.

2. E. J. Crane became the first Director of Chemical Abstracts Service when it became an American Chemical Society division in 1956. Crane had been CA editor since 1915, and his dedication was a key factor in its long-term success.

3. Dale B. Baker became the CAS Director upon Crane's retirement in 1958. According to CAS, his visionary view of CAS' potential "led to expansion, modernization, and the forging of international alliances with other information organizations." CAS was an early leader in the use of computer technology to organize and disseminate information.

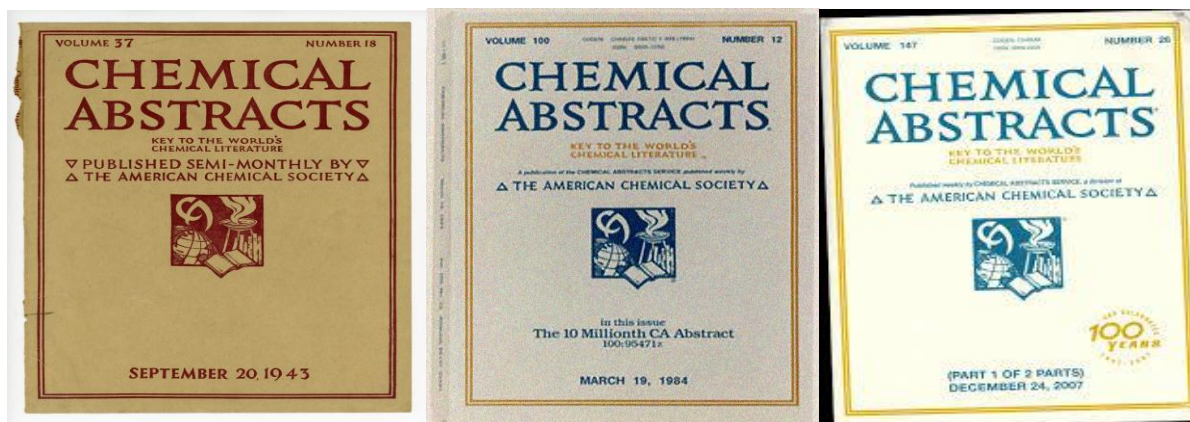


Figure 2: Chemical Abstracts Old & New.

The CAS Chemical Registry System was introduced in 1965. CAS developed a unique registry number to identify chemical substances. Agencies such as the U.S. Environmental Protection Agency and local fire departments around the world now rely on these numbers for the definite identification of substances. According to the ACS, this is the largest chemical substance database in the world. In 2007 the ACS designated its Chemical Abstracts Service subdivision an ACS National Historic Chemical Landmark in recognition of its significance as a comprehensive repository of research in chemistry and related sciences.

Committee on Chemical Abstracts Service (CAS)

The ACS Joint Board-Council Committee on Chemical Abstracts Service (CAS) duties include: Developing an informed, constructive and supportive relationship with the SOCIETY body established by the Board of Directors to manage and conduct the affairs of Chemical Abstracts Service, including reporting of each group's

activities to the other. Serving as a channel for information flow between the Governing Board for Publishing, SOCIETY members and individual Chemical Abstracts Service users to help assure that each party's needs and support are researched, recognized and appreciated. Encouraging and considering suggestions from the membership concerning CAS and transmitting these suggestions to the Governing Board for Publishing and the SOCIETY's Board of Directors. Responding to requests by the Governing Board for Publishing that will assist in furthering the Chemical Abstracts Service mission. Informing the Council and the Board of Directors of the Committee's activities.^[2]

Databases: The two principal databases that support the different products are **CAplus** and **Registry**.

CAplus: CAplus consists of bibliographic information and abstracts for all articles in chemical journals worldwide and chemistry-related articles from all

scientific journals, patents and other scientific publications. **CAplus - Worldwide coverage of many scientific disciplines all in one source.**

Benefit to you: 1. An integrated source of journal articles and patent documents in many scientific disciplines, including biomedical sciences, chemistry, engineering, materials science, agricultural science and more 2. English language summaries translated from the scientific literature published in more than 50 different languages from more than 180 different countries.

Content: CAplus, produced by CAS, contains more than 45 million chemistry and chemistry related research

records categorized in 80 sections, with references in: 1. All areas of **biochemistry:** Agrochemical regulators, Biochemical genetics, Fermentation, Immunochemistry, Pharmacology. 2. All areas of **organic chemistry:** Amino acids, Biomolecules, Carbohydrates, Organometallic compounds, Steroids. 3. All areas of **macromolecular chemistry:** Cellulose, lignin, paper, Coatings, inks, Dyes, organic pigments, Synthetic elastomers, Textiles, fibers. 4. All areas of **applied chemistry:** Air pollution, Ceramics, Essential oils, cosmetics, Fossil fuels, Ferrous metals, alloys. 5. All areas of **physical, inorganic, analytical chemistry:** Surface chemistry, Catalysts, Phase equilibrium, Nuclear phenomena, Electrochemistry.



Figure 3: American Chemical Society logo.

How do we count: CAplus covers international journals, patents, patent families, technical reports, books, conference proceedings, and dissertations from all areas of chemistry, biochemistry, chemical engineering and related sciences from 1907 to the present. In addition, over 180,000 records for pre-1907 patent and journal references are available, from sources such as the American Chemical Society (ACS), the Royal Society of Chemistry (RSC) and *Chemisches Zentralblatt*. Electronic-only journals and web preprints are also covered. Since October 1994, records for all articles from more than 1,500 key chemical journals are added, including records for document types not covered in Chemical Abstracts (CA): biographical items, book reviews, editorials, errata, letters to the editor, news announcements, product reviews, meeting abstracts and miscellaneous items. Cited references are included for journals, conference proceedings and basic patents from the USPTO, EPO, WIPO and German patent offices added to the CAS databases from 1997 to the present. Also included are patent examiner citations from British and French basic patents (2003 to the present), Canadian patents (2005 to the present) and Japanese patents (2011 to the present). In addition, nearly 300,000 existing patent records from 1982-2008 have been supplemented with information for cited patents. As of May 2017,

CAplus contains over 505 million cited references. Citing references are included when available. Legal status information is available for U.S. patents since 1980.^[3]

Coverage: Early 1800, Patent (and patent family) references from 63 patent authorities around the world. Chemistry indexed from more than 50,000 scientific journals worldwide, with thousands of active titles currently covered. From 1907 to present, CAS has indexed chemistry from more than 50,000 journal titles. In that time, publishers have discontinued, merged, split, revised and changed the focus of many titles, For more information about journal titles and abbreviations for publications indexed by CAS since 1907 please consult the CAS SOURCE INDEX (CASSI) search engine, Conference proceedings, Technical reports, Books, Dissertations, Reviews, Meeting abstracts, Electronic-only journals, Web preprints, Cover-to-cover coverage for more than 1500 key chemical journals (since October 1994), including records for document types not covered in *Chemical Abstracts* (CA), Biographical items, Books reviews, Editorials, Errata, Letters to the editor, News announcements, Product reviews, Meeting abstracts.



Figure 4: Chemical Abstracts Service Building B in August 2009. Columbus, Ohio.

Update frequency: Updated daily. Patent references from nine major issuing authorities available within two days from the time the patent was issued.

Registry: Registry contains information on more than 130 million organic and inorganic substances and more than 64 million protein and Nucleic acid sequences. The sequence information comes from CAS and Gen Bank, produced by the National Institutes of Health. The chemical information is produced by CAS and is prepared by the CAS Registry System, which identifies each compound with a specific CAS registry number, index name and graphic representation of its chemical structure. The assignment of chemical names is done according to the chemical nomenclature rules for CA index names, which is slightly different from the internationally standard IUPAC names, according to the rules of IUPAC.

Products: CAS databases are available via two principal database systems, STN and SciFinder.

A CAS Registry Number, also referred to as CASRN or CAS Registry Number, is a unique numerical identifier assigned by the Chemical Abstracts Service (CAS) to every chemical substance described in the open scientific literature (currently including those described from at least 1957 through the present), including organic and inorganic compounds, minerals, isotopes, alloys and nonstructurable materials (UVCBs, of unknown, variable composition, or biological origin). The Registry maintained by CAS is an authoritative collection of disclosed chemical substance information. It currently identifies more than 129 million organic and inorganic substances and 67 million protein and DNA sequences, plus additional information about each substance. It is updated with around 15,000 additional new substances daily.

Use: Historically, chemicals have been identified by a wide variety of synonyms. Frequently these are arcane and constructed according to regional naming conventions relating to chemical formulae, structures or origins. Well-known chemicals may additionally be known via multiple generic, historical, commercial and/or black-market names.

CAS Registry Numbers are simple and regular, convenient for database searches. They offer a reliable, common and international link to every specific substance across the various nomenclatures and disciplines used by branches of science, industry and regulatory bodies. Almost all molecule databases today allow searching by CAS Registry Number. On the other hand, CASRNs are not related to chemistry, are proprietary and unrelated to any previous systems and do not readily form phonetic analogs or synonyms.^[4]

Format: A CAS Registry Number has no inherent meaning but is assigned in sequential, increasing order when the substance is identified by CAS scientists for inclusion in the CAS REGISTRY database. A CASRN is separated by hyphens into three parts, the **first** consisting from two up to **seven** digits, the **second** consisting of **two** digits and the **third** consisting of a **single** digit serving as a check digit. The check digit is found by taking the last digit times 1, the previous digit times 2, the previous digit times 3 etc., adding all these up and computing the sum modulo 10. For example, the CAS number of water is 7732-18-5: the checksum 5 is calculated as $(8 \times 1 + 1 \times 2 + 2 \times 3 + 3 \times 4 + 7 \times 5 + 7 \times 6) = 105$; $105 \text{ mod } 10 = 5$.

Check Digit Verification of CAS Registry Numbers: A CAS Registry Number[®] includes up to 10 digits which are separated into 3 groups by hyphens. The first part of the number, starting from the left, has 2 to 7 digits; the second part has 2 digits. The final part consists of a single check digit. The check digit is developed by

following a standard calculation shown below. Use it to see if you have a valid CAS Registry Number. The CAS Registry Number may be written in a general form as:

$N_1 \dots N_4 N_3 - N_2 N_1 - R$; in which R represents the check digit and N represents a fundamental sequential number. The check digit is derived from the following formula: $(iN_1 + \dots + 4N_4 + 3N_3 + 2N_2 + 1N_1) \div 10 = Q + R/10$

In which Q represents an integer which is discarded. For example RN 107-07-03, the validity is checked as follows: $(5 \times 1 + 4 \times 0 + 3 \times 7 + 2 \times 0 + 1 \times 7) \div 10 = 33/10 = 3 + 3/10$ (3.3); Q=3 is discarded and R (check digit)=3.

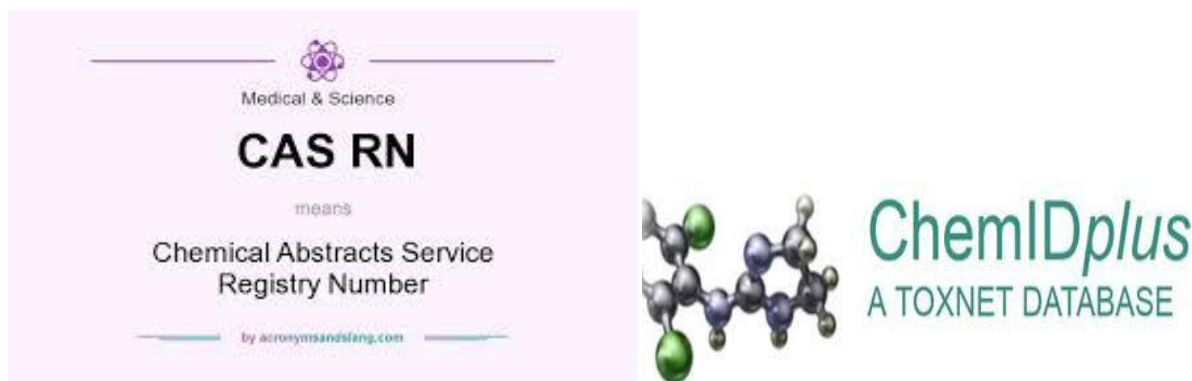


Figure 5: CAS RN & ChemIDplus database.

Granularity: Stereoisomers and racemic mixtures are assigned discrete CAS Registry Numbers: L-epinephrine has 51-43-4, D-epinephrine has 150-05-0 and racemic DL-epinephrine has 329-65-7. Different phases do not receive different CASRN (liquid water and ice both have 7732-18-5), but different crystal structures do (carbon in general is 7440-44-0, graphite is 7782-42-5 and diamond is 7782-40-3). Commonly encountered mixtures of known or unknown composition may receive a CASRN; examples are Leishman stain (12627-53-1) and mustard oil (8007-40-7). Some metals are discerned by their oxidation state, e.g. the element chromium has 7440-47-3, the trivalent Cr(III) has 16065-83-1 and the hexavalent Cr(VI) ion has 18540-29-9. Occasionally whole classes of molecules receive a single CASRN: the class of enzymes known as alcohol dehydrogenases has 9031-72-5.

Search engines: CHEMINDEX Search via Canadian Centre for Occupational Health and Safety, Chem ID plus Advanced via United States National Library of Medicine, Common Chemistry via Australian Inventory of Chemical Substances, European chemical Substances Information System via the website of Royal Society of Chemistry, HSNO Chemical Classification Information Database via Environmental Risk Management Authority, Search Tool of Australian Inventory of Chemical Substances.

What is CAS REGISTRY? CAS REGISTRYSM is the most authoritative collection of disclosed chemical substance information, containing more than 132 million organic and inorganic substances and 67 million sequences (view current numbers). CAS REGISTRY covers substances identified from the scientific literature from 1957 to the present, with additional substances going back to the early 1900s.^[5]

What is a CAS Registry Number (CAS RN)? Each CAS Registry Number[®] (CAS RN[®]) identifier: 1. Is a unique numeric identifier 2. Designates only one substance 3. Has no chemical significance 4. Is a link to a wealth of information about a specific chemical substances.

What does a CAS Registry Number look like? A CAS Registry Number is a numeric identifier that can contain up to 10 digits, divided by hyphens into three parts. The right-most digit is a check digit used to verify the validity and uniqueness of the entire number. For example, 58-08-2 is the CAS Registry Number for caffeine.

How does CAS assign Registry Numbers? A CAS Registry Number is assigned to a substance when it enters the CAS REGISTRY database. Numbers are assigned in sequential order to unique, new substances identified by CAS scientists for inclusion in the database.

What kinds of compounds does the CAS REGISTRY contain? CAS REGISTRY contains a wide variety of substances, including the world's largest collection of: Organic compounds, Inorganic compounds, Metals Alloys, Minerals, Coordination compounds, Organometallics, Elements, Isotopes, Nuclear particles, Proteins and nucleic acids, Polymers, Nonstructurable materials (UVCBs).

How frequently is the CAS REGISTRY database updated? Approximately 15,000 new substances are added each day.

Why have CAS Registry Numbers become the world standard? Since CAS Registry Numbers are not dependent upon any system of chemical nomenclature, they can: Provide a reliable common link between the various nomenclatures terms used to describe substances.

Serve as an international resource for chemical substance identifiers used by scientists, industry and regulatory bodies.

Why do regulatory agencies rely on CAS Registry Numbers? Chemical compounds can be described in many different ways: Molecular formula, Structure diagram, Systematic names, Generic names, Proprietary or trade names, Trivial names.

A CAS Registry Number, however, is unique and specific to only one substance regardless of how many other ways the substance can be described. Governmental agencies have found CAS Registry Numbers ideal for keeping track of substances because. They are unique, they can be validated quickly and reliably, they are internationally recognized.

Where can I find CAS REGISTRY Numbers? Find CAS Registry Numbers in: SciFinder[®], STN[®] databases, CAS publications, Other publications, Governmental regulatory agency commercial chemical inventories, Selected Elsevier databases, Handbooks, guides and technical reports, Other printed reference works, Chemical catalogs, *Why do some substances in CAS REGISTRY have zero references?* How can I learn more about these substances? Records in REGISTRY represent substances indexed for the CAS databases (CASM/CAPLUSSM, CASREACT[®], CHEMCATS[®], CHEMLIST[®], MARPAT[®]) and other databases in products such as SciFinder[®] and STN[®]. Substances that come from sources other than literature or patent publications may not contain any references. CAS indexes these substances to support registration policies, chemical libraries, chemical catalogs, web sources, reaction databases and data collections not represented in STN. To learn more about a substance in REGISTRY that does not have any literature or patent references consult the Source of Registration (SR) and Class Identifier (CI) fields in STN.

Why is it important to come to CAS for Registry Numbers? While printed publications may contain outdated information, the CAS REGISTRY database is updated daily providing your best source for the latest CAS Registry Number information. CAS is the source and final authority for CAS Registry Numbers. Other resources may have associated an incorrect CAS Registry Number with a compound and use of that incorrect CAS Registry Number in searches could lead you to irrelevant or inappropriate information.

What is the CAS RN Verified Partner Program? A CAS Registry Number license is required anytime an organization will "publish" CAS Registry Numbers to the public or use them to support features of a platform that is publicly or commercially available.^[6]

How can I obtain or request assignment of a CAS Registry Number? CAS Client Services offers you several options for confirming and assigning CAS Registry Numbers and obtaining CA Index Names. Note that there is a fee associated with this service.

CHEMINDEX Search via Canadian Centre for Occupational Health and Safety. Enter a Chemical Name or CAS Registry Number to see if that chemical is listed in Web Information Service. Click on "Synonyms" to see the various chemical names for that substance (free service).

<http://ccinfolweb.ccohs.ca/chemindex/search.html>

ChemIDplus Advanced via United States National Library of Medicine,
<https://chem.nlm.nih.gov/chemidplus/>

Common Chemistry via Australian Inventory of Chemical Substances.
<https://sis.nlm.nih.gov/chemical.html>

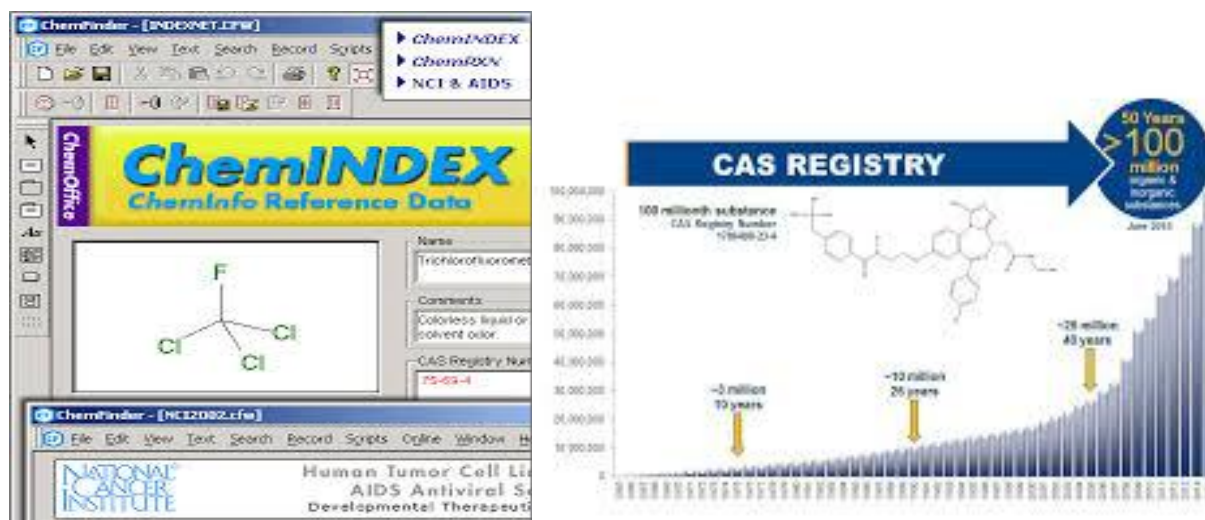


Figure 6: ChemIndex & CAS Registry database.

European chemical Substances Information System via the website of Royal Society of Chemistry. HSNO Chemical Classification Information Database via Environmental Risk Management Authority. Search Tool of Australian Inventory of Chemical Substances. CAS provides accurate and authoritative chemistry content, curated and quality-controlled by hundreds of Ph.D. scientists from around the world. CAS content covers all disclosed chemistry and related science from thousands of journals and 63 patent authorities, as well as reputable Web sources, dissertations, books, conference proceedings, chemical suppliers and more. Our information products, including SciFinder[®] and STN[®], are powerful and convenient ways to access the content CAS uses to create the following databases:

CAS REGISTRYSM - with more than 132 million small molecules (view latest numbers), is the gold standard for chemical substance information, including chemical structures, names, predicted and experimental properties, tags and spectra.

CAPLUSSM - includes more than 45 million records from the early 1800s to the present.

Chemical Abstracts Plus (CAPLUS) provides current and comprehensive worldwide coverage of chemistry and

related scientific disciplines. CAPLUS covers international journals, patents, patent families, technical disclosures, technical reports, books, conference proceedings, dissertations, electronic-only journals and web preprints from all areas of chemistry, biochemistry, chemical engineering and related sciences from 1907 to the present.

Cited references are included for journals, conference proceedings, and basic patents from the US, EPO, WIPO and German patent offices added to the CAS databases from 1997 to the present. In addition, nearly 300,000 existing patent records from 1982-2008 have been supplemented with information for cited patents. Bibliographic information and available abstracts for the articles from nearly 1,500 key chemical journals are added within 1 week of journal receipt. CAPLUS is updated daily with new bibliographic records and weekly with indexing.^[7]

File Data: 1907 to the present, plus more than 180,000 pre-1907 records, More than 45 million records (3/17), Updated daily with about 5,000 new citations, Updated weekly with indexing for approximately 12,000-16,000 records.

Substance Detail | Get References | Get Reactions | Get Commercial Sources | Get Regulatory Info | Send to SciPlanner

Link | Save | Print | Export

CAS Registry Number: 327-97-9
C₁₆H₁₈O₉
Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propen-1-yl]oxy]-1,4,5-trihydroxy-, (1S,3R,4R,5R)-
Chlorogenic acid (8CI); Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, (1S,3R,4R,5R)- (9CI); Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, [(1S-(1α,3β,4α,5α))]; 3-(3,4-Dihydroxycinnamoyl)quinic acid; 3-Caffeoylquinic acid; 3-O-(3,4-Dihydroxycinnamoyl)-D-quinic acid; 3-O-Caffeoylquinic acid; Heriguard; NSC 407296; NSC 70861
Deleted CAS Registry Numbers: 12626-41-4, 15076-00-3, 16310-14-8, 16431-25-7, 16431-26-8, 108657-60-9
Source of Registration: CA
~13,118 References
Document Types: Conference, Dissertation, Journal, Patent, Report

Absolute stereochemistry, Double bond geometry unknown.

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<input type="checkbox"/> Biotechnology	<input type="checkbox"/> Engineering & Construction	<input type="checkbox"/> Mathematics & Computer Science
<input type="checkbox"/> Business (Scientific & Technical)	<input type="checkbox"/> Environment Research & Technology	<input type="checkbox"/> Multidisciplinary Science & Technology
<input type="checkbox"/> Chemistry	<input type="checkbox"/> Geosciences	<input type="checkbox"/> Physics
<input type="checkbox"/> Social Sciences		

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Figure 7: CASR & STN.

Subject Coverage: All areas of chemistry and chemical engineering. The major subdivisions are: Applied Chemistry and Chemical Engineering, Biochemistry, Macromolecular Chemistry, Organic Chemistry, Physical, Inorganic and Analytical Chemistry

Sources: Cover-to-cover coverage of more than 1,500 key chemical journals since October 1994. Thousands of journals monitored, Patents, Technical disclosures, Conference proceedings, Technical reports, Books,

Dissertations, Reviews, Meeting abstracts, Web preprints, Electronic-only journals, Database Producer.

Chemical Abstracts Service: P.O. Box 3012, Columbus, Ohio 43210-0012 USA, Phone: 614-447-3700, Fax: 614-447-3751.

CASREACT[®] - chemical reaction database, includes more than 98.5 million reactions and synthetic preparations. **Benefit to you:** Access precise, dependable

and timely information on synthetic organic research, including organometallics, total syntheses of natural products and biotransformation reactions.

Answer questions such as:

- Different reactions producing the same product, - Uses or applications of a particular catalyst, - Various ways to carry out specific functional group transformations.

Content: CASREACT[®], produced by CAS, contains: More than 84.2 million single- and multi-step reactions -- available with SciFinder and on STN. More than 14.2 million additional synthetic preparations available with SciFinder.

How do we count: CASREACT consists of single- (A->B, B->C, C->D) and multi-step (A->C, A->D, B->D) reactions, plus synthetic preparations. Single- and multi-step reactions can be found in all CAS and STN products. Synthetic preparations are accessible through the SciFinder Explore Reactions function or by applying a product role limiter on a CAS Registry Number search in STN.^[8]

Coverage: 1840 to the present.

CASREACT contains reaction information from the millions of published journal articles and patent documents selected for inclusion in Chemical AbstractsTM (CA).

Update frequency: Updated daily, More than 150,000 single- and multi-step reactions are added each week, Sample record from SciFinder, Reaction display with experimental procedure information in SciFinder.

CHEMCATS[®] - provides access to millions of commercially available chemicals from hundreds of suppliers

Benefit to you: The next time you have to order chemicals, you can quickly find the substances you need thanks to CHEMCATS[®]. You will find the following information (depending on the supplier): Catalog name, Order number, Chemical and trade names, CAS Registry Number[®], Chemical structure, Pricing terms.

Supplier contact information: Company name and address, Phone and fax number, E-mail, Web address.

Content: CHEMCATS (Chemical Catalogs Online), produced by CAS, is a catalog database containing information about commercially available chemicals and their worldwide suppliers.

How do we count: CHEMCATS consists of commercially available products. Products listed by vendors as different catalog items may reflect various factors, such as purity, grade, or quantity.

Coverage: Current catalogs and chemical libraries.

Update frequency: Updated at least two times per week with new and revised catalog information.

CHEMLIST[®] - worldwide regulated chemicals database contains more than 348,000 substances.

Benefit to you: You can quickly locate the regulatory information you need because each substance reference provides all the agencies - international, national and state - that regulate the substance.

Content: CHEMLIST[®] (Regulated Chemicals Listing), produced by CAS, is an electronic collection of thousands of chemical substances that are regulated in key markets across the globe. CHEMLIST contains more than 348,000 substances.

How do we count: The CHEMLIST database began with national chemical inventories such as Toxic Substances Control Act (TSCA), European Inventory of Existing Commercial Chemical Substances (EINECS), Existing and New Chemical Substances (ENCS) and Inventory of Existing Chemical Substances in China (IECSC). Today, it includes international lists for high production volume (HPV) chemicals, priority chemicals, dangerous chemicals with transportation restrictions, as well as pollutant release inventories. CHEMLIST offers the convenience of identifying--in one place--the regulatory requirements for a specific substance from many of the world's most significant regulated substances lists.

Coverage: Inventories and lists from 1980 to the present.

Update frequency: More than 50 new substances or additions to existing substances are added to the database each week.

CIN[®] - Chemical Industry Notes covers more than 1.7 million worldwide chemical business news citations from 1974 to the present.

Benefits to you: When you need current business news related to production, pricing, sales, facilities, products and processes, or corporate and government activities, you can find it in Chemical Industry Notes (CIN[®]).

Content: CIN, produced by CAS, contains records extracted from chemical industry trade publications.

Currently, CIN has more than 1.7 million records, including Bibliographic information, Abstracts and indexing, CAS Registry Numbers[®].

Coverage: 1974 to present.

Sources include: Government publications, Journals, Newsletters, Newspapers, Special reports, Trade magazines.

Update frequency: Weekly, Weekly and biweekly alerts (SDIs) are available.

How do we count: Counts the abstracts added from the sources indexed in Chemical Industry Notes related to production, pricing, sales, facilities, products and processes, corporate activities, government activities, and people

MARPAT[®] - this structure searchable database includes more than 1,162,000 generic Markush structures.^[9]

STN: STN[®] Database Summary Sheets (DBSS) provide information you need to use the databases on STN. Each sheet describes the content, sources, file data and producer. Each also includes search fields and examples, display fields and formats and a sample record that allows you to see the way information is presented in the database.

STN (Scientific & Technical Information Network) International is operated jointly by CAS and FIZ Karlsruhe and is intended primarily for information professionals, using a command language interface. In addition to CAS databases, STN also provides access to many other databases, similar to Dialog.

SciFinder



Figure 8: SciFinder.

SciFinder is a database of chemical and bibliographic information. Originally a client application, a web version was released in 2008. It has a graphics interface, and can be searched for chemical structures and reactions. SciFinder[®] is a research discovery application that provides unlimited access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences. SciFinder offers a one-stop shop experience with flexible search and discover options based on user input and workflow. You can search for substances, reactions and patent and journal references anytime, anywhere. Make better, more confident decisions knowing that you have access to the largest collection of substances, reactions and patent and journal references produced, compiled and updated daily by CAS scientists around the world. Save time with an array of powerful

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Proven Reliability: STN goes beyond content and tools. As your partner with more than 30 years of dedicated service to professional searchers, we care about the quality of your search results and are ready to help when you need us.^[10]

tools to search, filter, analyze and plan that allow you to quickly find the most relevant answers to your research questions. Don't worry about missing vital research - if it's publically disclosed, high quality and from a reliable source, SciFinder has it! See why industry experts rely on SciFinder as their only source for high-quality content combined with ease-of-use features that help complete their research project from start to finish. And now with PatentPak[®], a robust, new patent workflow solution which offers instant access to hard-to-find chemistry in full-text patents directly in SciFinder.

The client version is for chemists in commercial organizations. Versions for both the Windows and Macintosh exist. SciFinder Scholar is for universities and other academic institutions and lacks some supplementary features for multi-database searching.

CASSI: CASSI stands for Chemical Abstracts Service Source Index. Since 2009 this formerly prints and CD-ROM compilation is available as a free online resource to look up and confirm publication information. The online CASSI Search Tool provides titles and abbreviations, CODEN, ISSN, publisher and date of first issue (history) for a selected journal. Also included is its

language of text and language of summaries. The range is from 1907 to the present, including both serial and non-serial scientific and technical publications. The database is updated quarterly. Beyond CASSI lists abbreviated journal titles from early chemical literature and other historical reference sources.^[11]

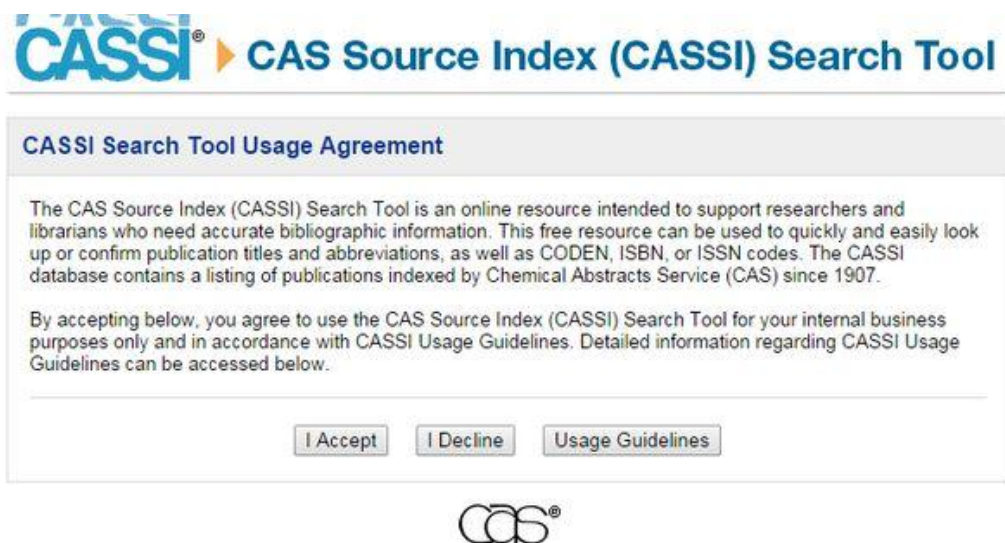


Figure 9: CASSI.

CONCLUSION

Every chemical is assigned a CAS number. Have you ever wondered what a CAS number is and how they are assigned? Check out this very simple explanation that will give you everything you need to know about what a CAS number is and how it's assigned to each chemical.

THE CHEMICAL ABSTRACT SERVICE OR CAS

The Chemical Abstract Service is part of the American Chemical Society and maintains a database of chemical compounds and sequences. The CAS database currently contains over 55 million different organic and inorganic chemical compounds. Each CAS entry is identified by their CAS Registry Number or CAS Number for short.

CAS NUMBERS

CAS Numbers are up to 10 digits long using the format xxxxxx-yy-z. They are assigned to a compound as the CAS registers a new compound. The number has no significance to the chemistry, structure or chemical nature of the molecule. The CAS Number of a compound is a useful way to identify a chemical over its name. For example, the compound CAS 64-17-5 refers to ethanol. Ethanol is also known as ethyl alcohol, ethyl hydrate, absolute alcohol, grain alcohol, hydroxyethane. The CAS number is the same for all these names. The CAS Number can also be used to distinguish between stereoisomers of a compound. Glucose is a sugar molecule that has two forms: D-glucose and L-glucose. D-glucose is also called dextrose and has CAS number 50-99-7. L-glucose is the mirror image of D-glucose and has a CAS Number of 921-60-8.

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