

COMPOUND SUMMARY

Sodium decanoate

[Cite](#) [Download](#)

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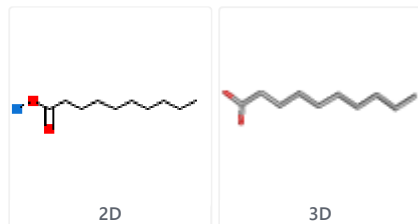
12 Patents

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14 Information Sources

PubChem CID: 4457968

Structure:

[Find Similar Structures](#)Molecular Formula: C₁₀H₁₉NaO₂

Chemical Names:

Sodium decanoate
Sodium caprate
1002-62-6
Decanoic acid, sodium salt
Decanoic acid sodium salt[More...](#)

Molecular Weight: 194.25 g/mol

Dates:

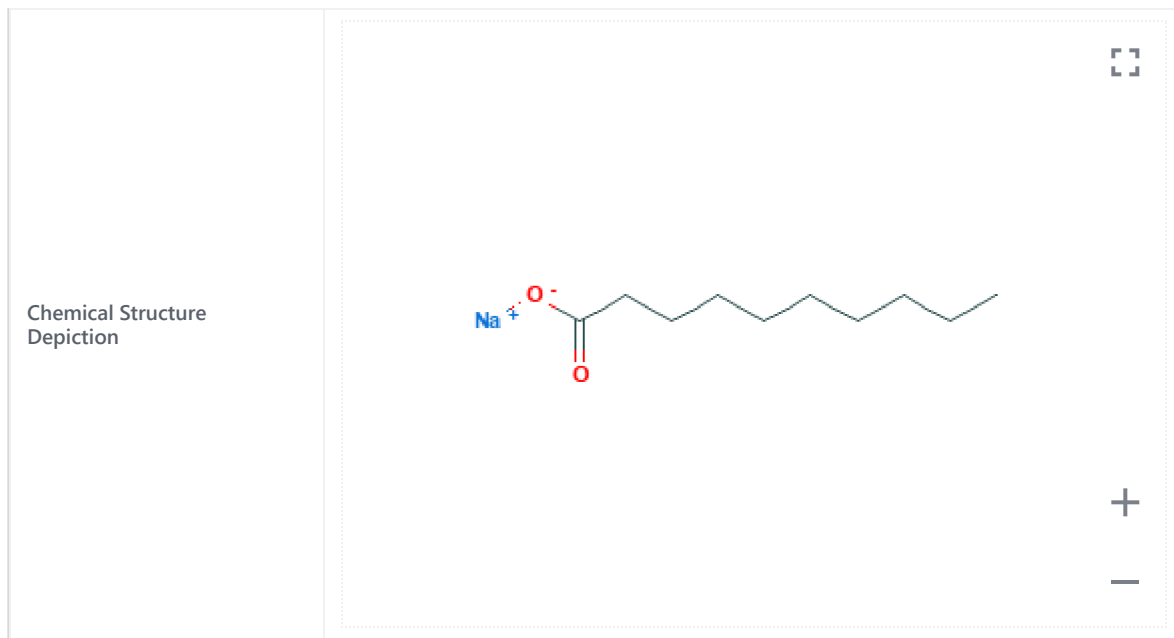
Modify: 2019-08-24
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1 Structures



1.1 2D Structure

[Find Similar Structures](#) [Get Image](#) [Download](#)



▶ from PubChem

1.2 3D Conformer



3D Conformer of Parent

▶ [from PubChem](#)

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

sodium;decanoate

▶ [from PubChem](#)

2.1.2 InChI

InChI=1S/C10H20O2.Na/c1-2-3-4-5-6-7-8-9-10(11)12;/h2-9H2,1H3,(H,11,12);/q;+1/p-1

▶ [from PubChem](#)

2.1.3 InChI Key

FIWQZURFGYXCEO-UHFFFAOYSA-M

▶ [from PubChem](#)

2.1.4 Canonical SMILES

CCCCCCCCC(=O)[O-].[Na+]

▶ [from PubChem](#)

2.2 Molecular Formula

C₁₀H₁₉NaO₂

▶ [from PubChem](#)

2.3 Other Identifiers

2.3.1 CAS

1002-62-6

▶ from ChemIDplus; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA)

Related CAS

334-48-5 (Parent)

▶ from ChemIDplus

2.3.2 European Community (EC) Number

213-688-4

▶ from European Chemicals Agency (ECHA)

2.3.3 UNII

4I820XKV2A

▶ from FDA/SPL Indexing Data

2.3.4 Wikipedia

Sodium caprate

▶ from Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

capric acid
decanoic acid
decanoic acid, sodium salt

sodium caprate
sodium decanoate

▶ from MeSH

2.4.2 Depositor-Supplied Synonyms



Sodium decanoate	EINECS 213-688-4	SCHEMBL29096	TR-000096
Sodium caprate	n-Capric acid sodium salt	DTXSID0027351	D0024
1002-62-6	4I820XKV2A	CTK8A8969	ST51037184
Decanoic acid, sodium salt	MFCD00066453	FIWQZURFGYXCEO-UHFFFAOYSA-M	MFCD00066453
Decanoic acid sodium salt	SodiumDecanoate	KS-000015YC	J-000080
Sodium caprylate	C10H19O2.Na	ANW-14204	UNII-6H91L1NXT
Sodium-n-decanoate	potassium decoate	AKOS015839877	UNII-RITQH25F4
Sodium decanoic acid	sodiumdecanoicacid	MCULE-2720595773	
Capric acid sodium salt	sodium n-decanoate	RTR-000096	
Capric acid, sodium salt	capricacidsodiumsalt	AK130453	
Caprinic acid sodium salt	AC1NAURY	AN-19640	
Decanoic acid, sodium salt (1:1)	ACMC-2097ny	LS-59381	
UNII-4I820XKV2A	n-decanoic acid sodium salt	SY104388	

▶ from PubChem

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value
Molecular Weight	194.25 g/mol
Hydrogen Bond Donor Count	0
Hydrogen Bond Acceptor Count	2
Rotatable Bond Count	8
Exact Mass	194.128274 g/mol
Monoisotopic Mass	194.128274 g/mol
Topological Polar Surface Area	40.1 A ²

Property Name	Property Value
Heavy Atom Count	13
Formal Charge	0
Complexity	116
Isotope Atom Count	0
Defined Atom Stereocenter Count	0
Undefined Atom Stereocenter Count	0
Defined Bond Stereocenter Count	0
Undefined Bond Stereocenter Count	0
Covalently-Bonded Unit Count	2
Compound Is Canonicalized	Yes

▶ from PubChem

3.2 Experimental Properties



3.2.1 Physical Description



Liquid

▶ from EPA Chemicals under the TSCA

4 Spectral Information



4.1 1D NMR Spectra



4.1.1 1H NMR Spectra



Instrument Name	Varian CFT-20
Copyright	Copyright © 2009-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	



▶ from SpectraBase

4.1.2 ¹³C NMR Spectra



Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ from SpectraBase

4.2 IR Spectra



4.2.1 FTIR Spectra



Technique	FILM (CAST FROM METHANOL)
Source of Sample	Chem Service, Inc., West Chester, Pennsylvania
Catalog Number	S-00030
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ from SpectraBase

5 Related Records



5.1 Related Compounds with Annotation



▶ from PubChem

5.2 Parent Compound



2969

▶ from PubChem

5.3 Related Compounds



Same Connectivity	3 Records
Same Parent, Connectivity	252 Records
Same Parent, Exact	234 Records
Mixtures, Components, and Neutralized Forms	2 Records
Similar Compounds	303 Records

▶ from PubChem

5.4 Substances



5.4.1 Related Substances



Same	59 Records
------	----------------------------

▶ from PubChem

5.4.2 Substances by Category



▶ from PubChem

6 Chemical Vendors



▶ from PubChem

7 Food Additives and Ingredients ?

7.1 FDA Substances Added to Food ?

Substance	SODIUM CAPRATE
Used for (Technical Effect)	LUBRICANT OR RELEASE AGENT
Document Number (21 CFR)	172.863

▶ from FDA Center for Food Safety and Applied Nutrition (CFSAN)

8 Pharmacology and Biochemistry ?

8.1 MeSH Pharmacological Classification ?


Antifungal Agents

Substances that destroy fungi by suppressing their ability to grow or reproduce. They differ from FUNGICIDES, INDUSTRIAL because they defend against fungi present in human or animal tissues. (See [all compounds classified as Antifungal Agents](#).)

▶ from MeSH

9 Use and Manufacturing ?

9.1 Use Classification ?

EPA Safer Chemical Functional Use Classes	Surfactants
Safer Chemical Classes	 Green circle - The chemical has been verified to be of low concern

▶ from EPA Safer Choice

9.2 Uses ?

EPA CPDat Chemical and Product Categories

▶ from EPA Chemical and Products Database (CPDat)

9.2.1 Industry Uses



Surface active agents

<https://www.epa.gov/chemical-data-reporting>

▶ from EPA Chemicals under the TSCA

9.2.2 Consumer Uses



Cleaning and furnishing care products

<https://www.epa.gov/chemical-data-reporting>

▶ from EPA Chemicals under the TSCA

9.3 General Manufacturing Information



Industry Processing Sectors

All other basic organic chemical manufacturing

▶ [from EPA Chemicals under the TSCA](#)

EPA TSCA Commercial Activity Status

Decanoic acid, sodium salt (1:1): ACTIVE

<https://www.epa.gov/tsca-inventory>

▶ [from EPA Chemicals under the TSCA](#)

10 Safety and Hazards



10.1 Hazards Identification



10.1.1 EPA Safer Chemical



Chemical: Sodium decanoate



Green circle - The chemical has been verified to be of low concern based on experimental and modeled data.

▶ [from EPA Safer Choice](#)

11 Literature



11.1 NLM Curated PubMed Citations



▶ from PubChem

11.2 Springer Nature References



▶ from Springer Nature

11.3 Chemical Co-Occurrences in Literature



▶ from PubChem

11.4 Chemical-Disease Co-Occurrences in Literature



▶ from PubChem

11.5 Chemical-Gene Co-Occurrences in Literature



▶ from PubChem

12 Patents



12.1 Depositor-Supplied Patent Identifiers



▶ from PubChem

[Link to all deposited patent identifiers](#)

▶ from PubChem

13 Classification



13.1 Ontologies



13.1.1 MeSH Tree



▶ from MeSH

13.1.2 WIPO IPC



▶ from WIPO

13.1.3 EPA Safer Choice



▶ from EPA Safer Choice

13.1.4 ChemIDplus



▶ from ChemIDplus

13.1.5 EPA CPDat Classification



▶ from EPA Chemical and Products Database (CPDat)

14 Information Sources



FILTER BY SOURCE

ALL SOURCES



1. ChemIDplus

Sodium caprate

<https://chem.nlm.nih.gov/chemidplus/sid/0001002626>

ChemIDplus Chemical Information Classification

<https://chem.sis.nlm.nih.gov/chemidplus/>

2. EPA Chemicals under the TSCA

LICENSE

<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

Decanoic acid, sodium salt (1:1)

<https://www.epa.gov/chemicals-under-tsca>

3. EPA DSSTox

Sodium decanoate

<https://comptox.epa.gov/dashboard/DTXSID0027351>

4. European Chemicals Agency (ECHA)

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<https://echa.europa.eu/web/guest/legal-notice>

sodium decanoate

<https://echa.europa.eu/substance-information/-/substanceinfo/100.012.444>

5. EPA Chemical and Products Database (CPDat)

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<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

sodium decanoate

<https://comptox.epa.gov/dashboard/DTXSID0027351#exposure>

EPA CPDat Classification

<https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat>

6. EPA Safer Choice

Sodium decanoate

<https://www.epa.gov/saferchoice/safer-ingredients>

EPA Safer Chemical Ingredients Classification

<https://www.epa.gov/saferchoice>

7. FDA Center for Food Safety and Applied Nutrition (CFSAN)

SODIUM CAPRATE

<https://www.accessdata.fda.gov/scripts/fdcc/?set=FoodSubstances&id=SODIUMCAPRATE>

8. FDA/SPL Indexing Data

4I820XKV2A

<https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/>

9. **SpectraBase**

<https://spectrabase.com/spectrum/63q1hhyRYPt>

<https://spectrabase.com/spectrum/APbxv9UFHNw>

<https://spectrabase.com/spectrum/DtaU0Pcs9zE>

10. **Springer Nature**11. **Wikipedia**

sodium caprate

https://ru.wikipedia.org/wiki/%D0%9A%D0%B0%D0%BF%D1%80%D0%B8%D0%BD%D0%B0%D1%82_%D0%BD%D0%B0%D1%82%D1%80%D0%B8%D1%8F

12. **PubChem**

<https://pubchem.ncbi.nlm.nih.gov>

13. **MeSH**

decanoic acid

<https://www.ncbi.nlm.nih.gov/mesh/67031071>

MeSH Tree

<http://www.nlm.nih.gov/mesh/meshhome.html>

Antifungal Agents

<https://www.ncbi.nlm.nih.gov/mesh/68000935>

14. **WIPO**

International Patent Classification

<http://www.wipo.int/classifications/ipc/>