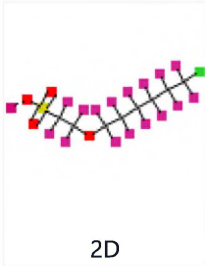
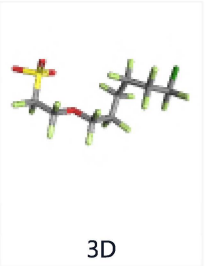


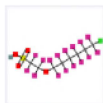


COMPOUND SUMMARY

Potassium 9-chlorohexadecafluoro-3-oxanonane-1-sulfonate

PubChem CID	25210512
Structure	<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  <p>2D</p> </div> <div style="text-align: center;">  <p>3D</p> </div> </div>
Molecular Formula	C₈ClF₁₆KO₄S
Synonyms	<p>73606-19-6</p> <p>Potassium 9-chlorohexadecafluoro-3-oxanonane-1-sulfonate</p> <p>2-[(6-Chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl)oxy]-1,1,2,2-tetrafluoroethanesulfonic acid,potassium salt</p> <p>SCHEMBL25286382</p> <p>DTXSID60881236</p> <p>View More...</p>
Molecular Weight	<p>570.67 g/mol</p> <p><i>Computed by PubChem 2.1 (PubChem release 2021.05.07)</i></p>
Parent Compound	<div style="display: flex; align-items: center;">  <div style="margin-left: 10px;"> <p>CID 22568738 (Perfluoro(2-((6-chlorohexyl)oxy)ethanesulfonic acid))</p> </div> </div>
Component Compounds	<div style="display: flex; align-items: center;">  <div style="margin-left: 10px;"> <p>CID 5462222 (Potassium)</p> </div> </div>



CID 22568738 (Perfluoro(2-((6-chlorohexyl)oxy)ethanesulfonic acid))

Dates

Create: 2009-04-09
Modify: 2024-04-27

Contents

Title and Summary

1 Structures ▼

2 Names and Identifiers ▼

3 Chemical and Physical Properties ▼

4 Related Records ▼

5 Chemical Vendors

6 Use and Manufacturing ▼

7 Literature ▼

8 Patents ▼

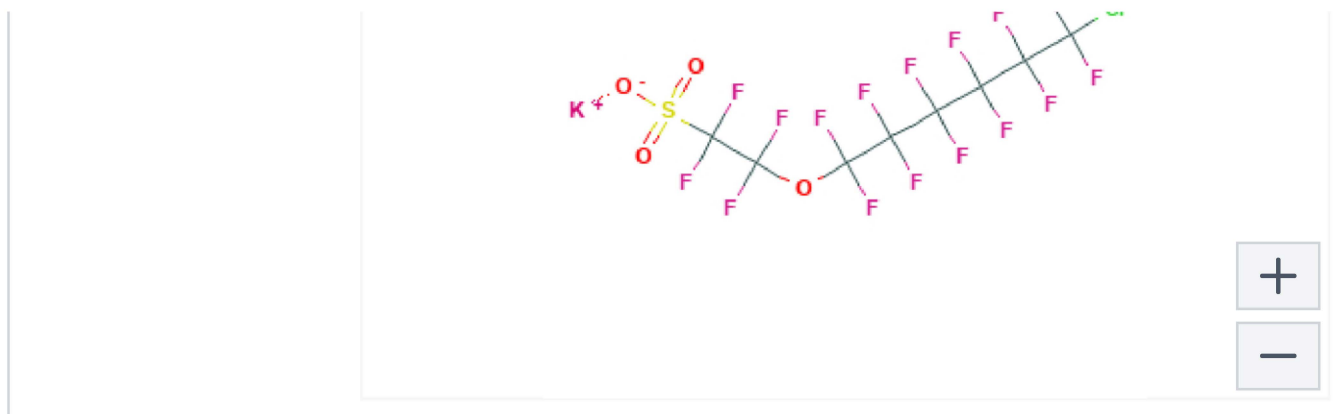
9 Classification ▼

10 Information Sources

1 Structures 🔍 🔗

1.1 2D Structure 🔍 🔗

Chemical Structure Depiction

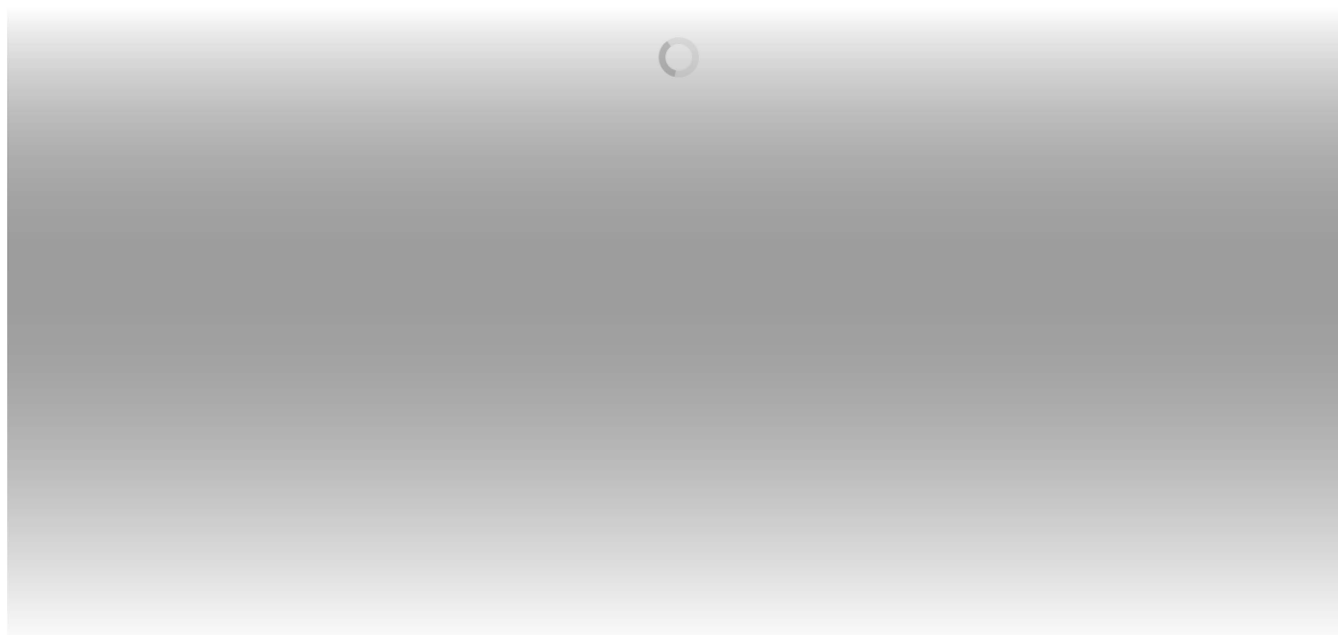


► PubChem

1.2 3D Conformer



3D Conformer of Parent



► PubChem

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



potassium;2-(6-chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexoxy)-1,1,2,2-tetrafluoroethanesulfonate

Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)

▶ [PubChem](#)

2.1.2 InChI



InChI=1S/C8HClF16O4S.K/c9-5(18,19)3(14,15)1(10,11)2(12,13)4(16,17)6(20,21)29-7(22,23)8(24,25)30(26,27)28;/h(H,26,27,28);/q;+1/p-1

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

▶ [PubChem](#)

2.1.3 InChIKey



OWQCHLFKOGVODW-UHFFFAOYSA-M

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

▶ [PubChem](#)

2.1.4 Canonical SMILES



C(C(C(C(F)(F)Cl)(F)F)(F)F)(C(C(OC(C(F)(F)S(=O)(=O)[O-])(F)F)(F)F)(F)F).[K+]

Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

▶ [PubChem](#)

2.2 Molecular Formula



C₈ClF₁₆KO₄S

Computed by PubChem 2.1 (PubChem release 2019.06.18)

▶ [PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



73606-19-6

▶ EPA DSSTox

2.3.2 Deprecated CAS



1464148-65-9

▶ EPA DSSTox

2.3.3 DSSTox Substance ID



DTXSID60881236

▶ EPA DSSTox

2.3.4 Nikkaji Number



J2.130.971K

▶ Japan Chemical Substance Dictionary (Nikkaji)

2.4 Synonyms



2.4.1 MeSH Entry Terms



2-((6-chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl)oxyl)-1,1,2,2-tetrafluoroethanesulfonic acid potassium salt

2-(6-chlorododecafluorohexyloxy)-1,1,2,2-tetrafluoroethanesulfonic acid potassium salt

9CI PF3ONS

9CIPF3ONS

potassium 9-chlorohexadecafluoro-3-oxanonane-1-sulfonate

potassium;2-(6-chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexoxy)-1,1,2,2-tetrafluoroethanesulfonate

▶ Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms



73606-19-6

Potassium 9-chlorohexadecafluoro-3-oxanonane-1-sulfonate

2-[(6-Chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl)oxy]-1,1,2,2-tetrafluoroethanesulfonic acid,potassium salt

SCHEMBL25286382

DTXSID60881236

OWQCHLFKOGVODW-UHFFFAOYSA-M

NS00019227

Potassium 2-((6-chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl)oxy)-1,1,2,2-tetrafluoroethanesulfonate

► [PubChem](#)

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	570.67 g/mol	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	20	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	9	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	569.8587394 g/mol	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	569.8587394 g/mol	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	74.8Å ²	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	31	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	762	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Isotope Atom Count	0	Computed by PubChem

Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	2	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2010.01.29)

► [PubChem](#)

3.2 Chemical Classes



3.2.1 PFAS



PFAS -> OECD Category

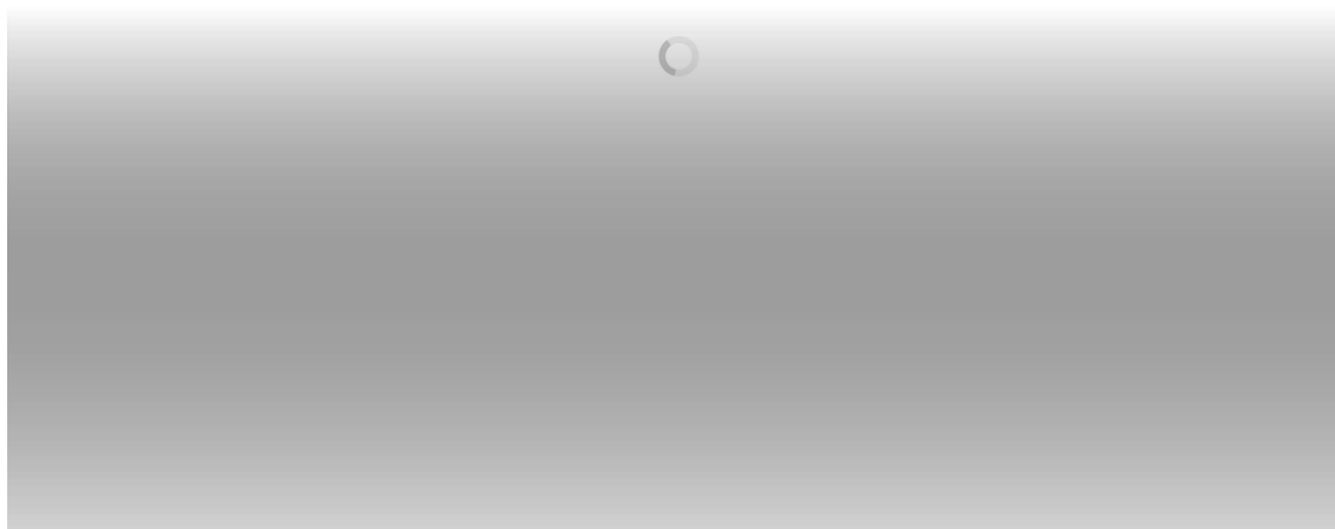
S25 | [OECDPFAS](#) | *List of PFAS from the OECD* | [DOI:10.5281/zenodo.2648775](https://doi.org/10.5281/zenodo.2648775)

► [NORMAN Suspect List Exchange](#)

4 Related Records

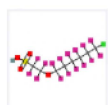


4.1 Related Compounds with Annotation



▶ PubChem

4.2 Parent Compound



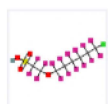
CID 22568738 (Perfluoro(2-((6-chlorohexyl)oxy)ethanesulfonic acid))

▶ PubChem

4.3 Component Compounds



CID 5462222 (Potassium)



CID 22568738 (Perfluoro(2-((6-chlorohexyl)oxy)ethanesulfonic acid))

▶ PubChem

4.4 Related Compounds



Same Parent, Exact Count	6
Mixtures, Components, and Neutralized Forms Count	2
Similar Compounds Count	7

▶ PubChem

4.5 Substances



4.5.1 Related Substances

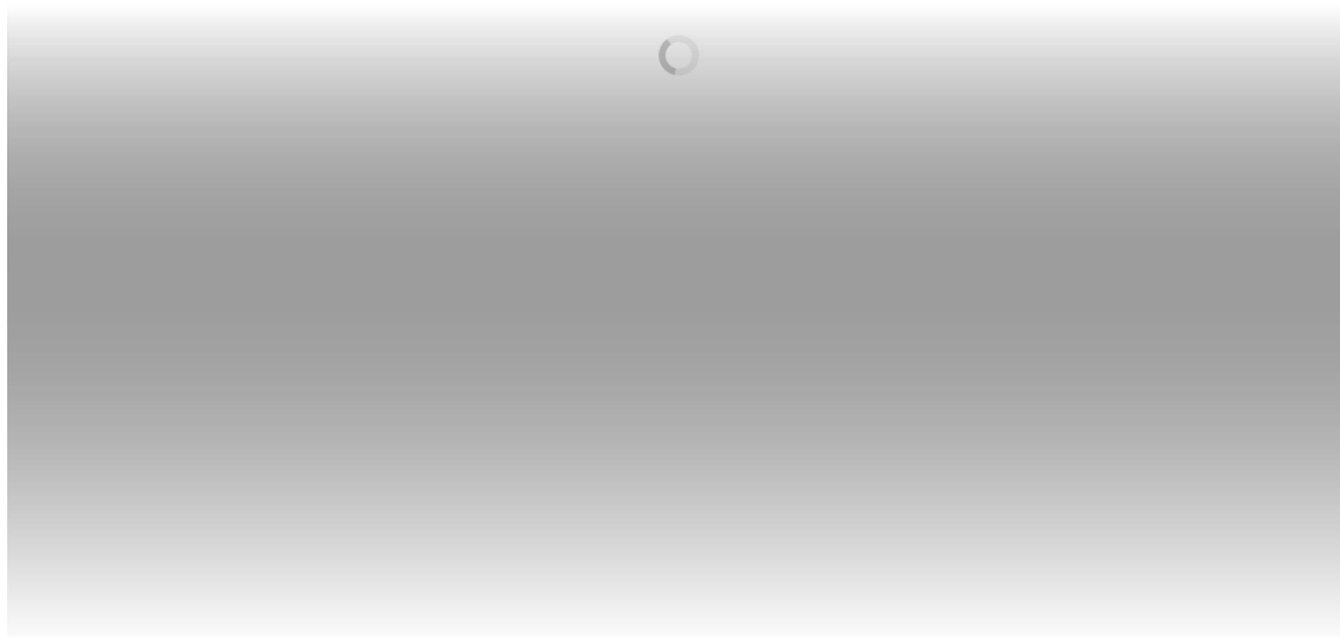


Same Count

20

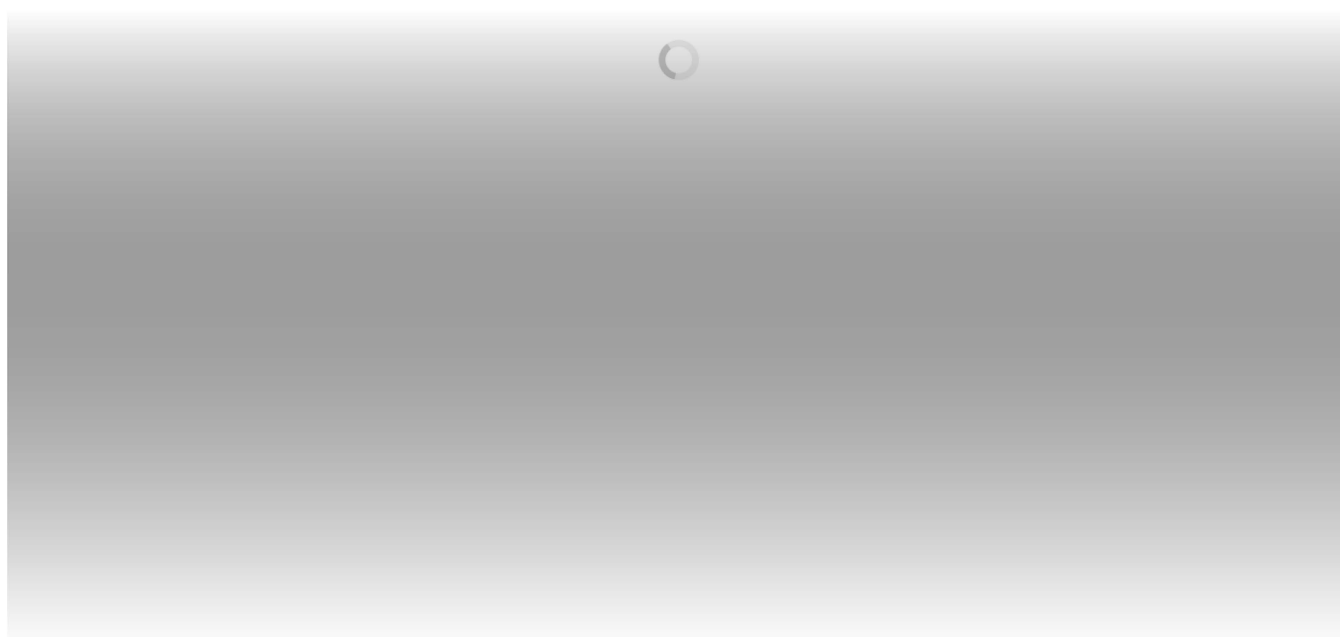
▶ PubChem

4.5.2 Substances by Category



▶ PubChem

5 Chemical Vendors



6 Use and Manufacturing



6.1 Uses



non-polymer PFAS -> Electroplating -> Chrome plating

non-polymer PFAS -> Energy Sector -> Continuous separation of **carbon dioxide** in flue gases

S80 | PFASGLUEGE | Overview of PFAS Uses | DOI:10.5281/zenodo.5029173

▶ **NORMAN Suspect List Exchange**

- Processing aid [Ref: CAS2019 (CN102504063)]
- Separating **carbon dioxide** in flue gas [Ref: CAS2019 (CN106914122)]
- Metal plating [Ref: <https://doi.org/10.1016/j.envint.2013.08.021>]

S80 | PFASGLUEGE | Overview of PFAS Uses | DOI:10.5281/zenodo.5029173

▶ **NORMAN Suspect List Exchange**

6.1.1 Use Classification



PFAS (per- and polyfluoroalkyl substances) -> OECD Category

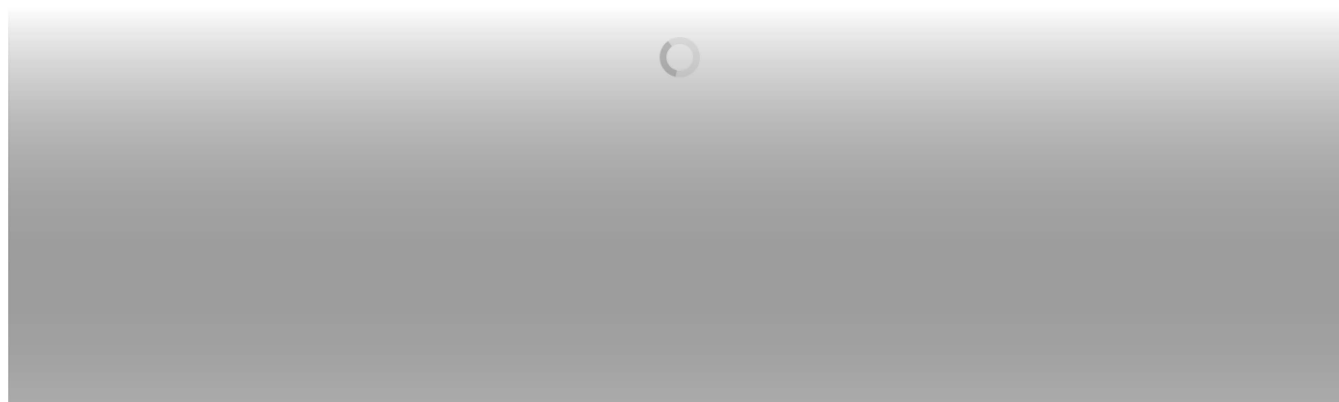
S25 | OECDPFAS | List of PFAS from the OECD | DOI:10.5281/zenodo.2648775

▶ **NORMAN Suspect List Exchange**

7 Literature

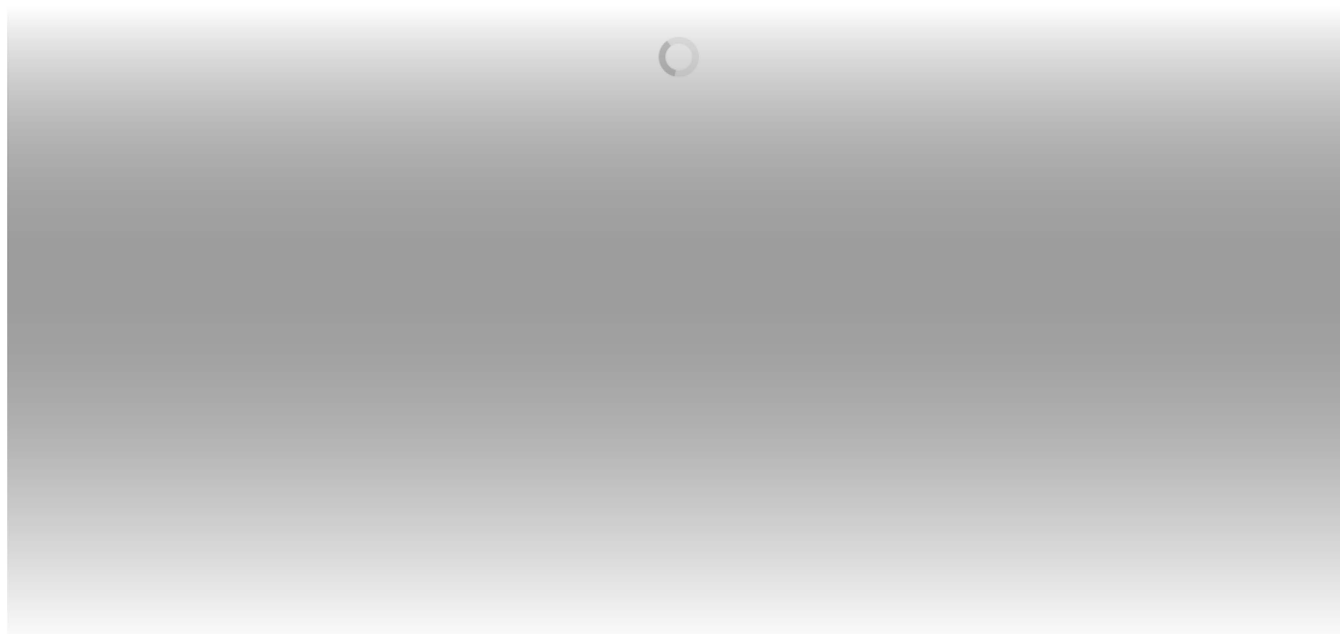


7.1 Consolidated References



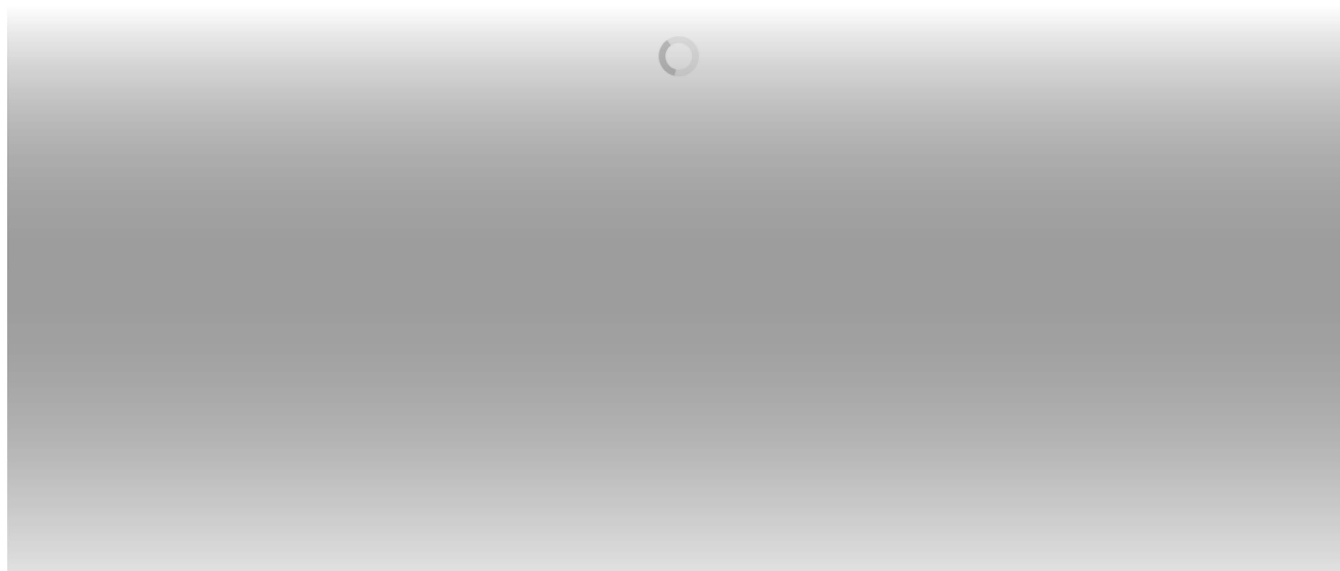
▶ PubChem

7.2 NLM Curated PubMed Citations



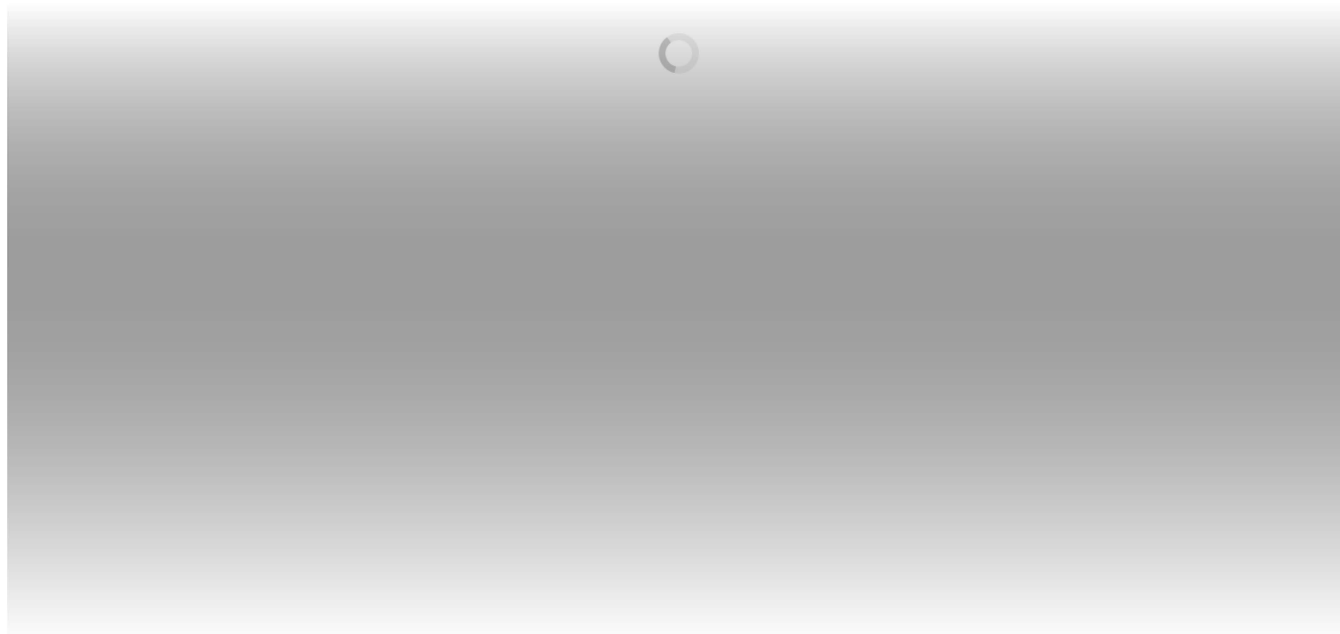
▶ PubChem

7.3 Springer Nature References



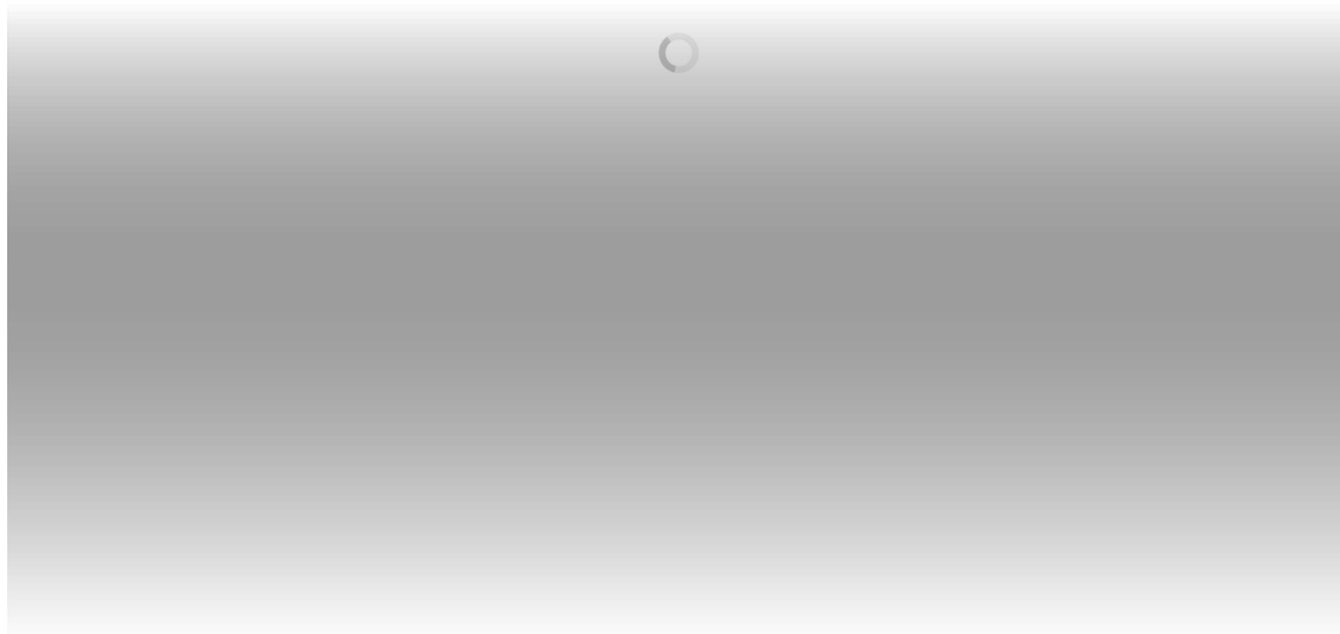
▶ Springer Nature

7.4 Chemical Co-Occurrences in Literature

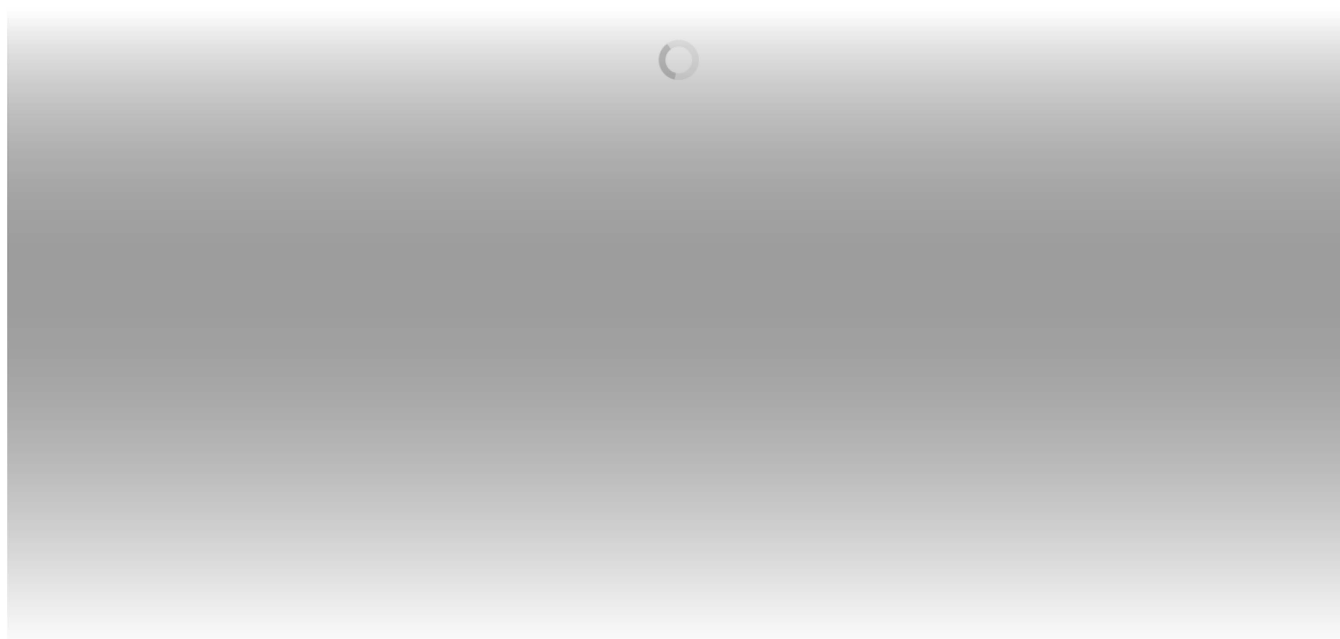


▶ PubChem

7.5 Chemical-Gene Co-Occurrences in Literature



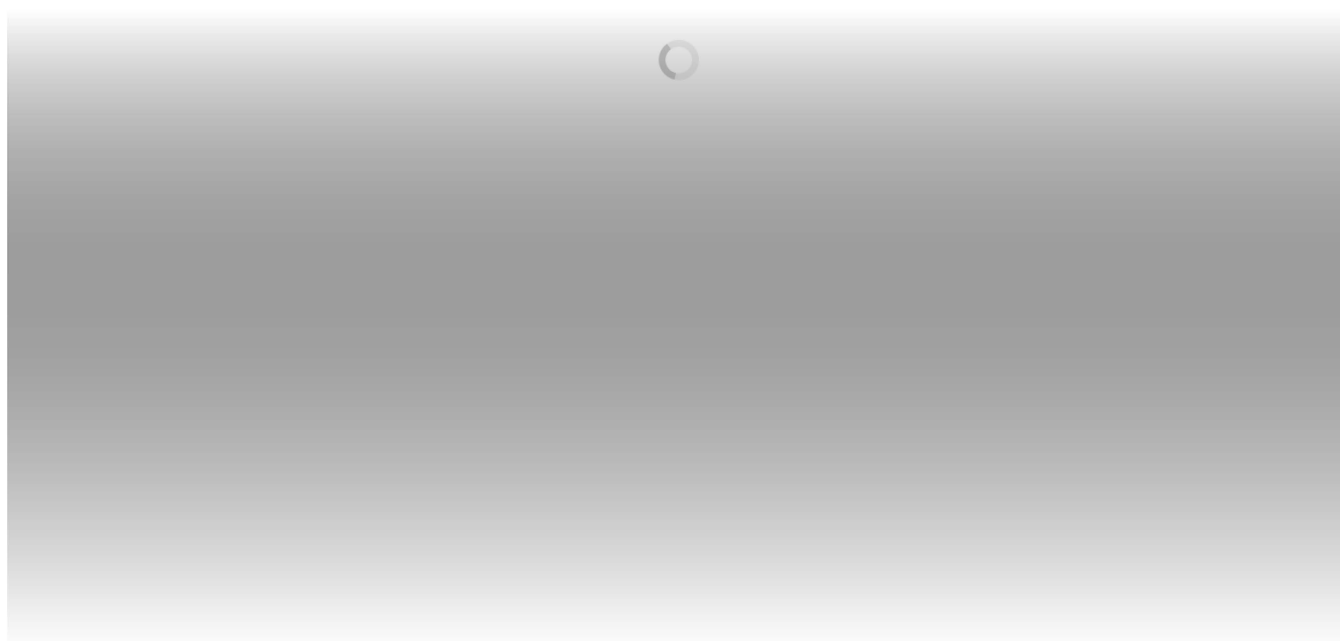
7.6 Chemical-Disease Co-Occurrences in Literature



8 Patents



8.1 Depositor-Supplied Patent Identifiers



▶ PubChem

[Link to all deposited patent identifiers](#)

▶ PubChem

8.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

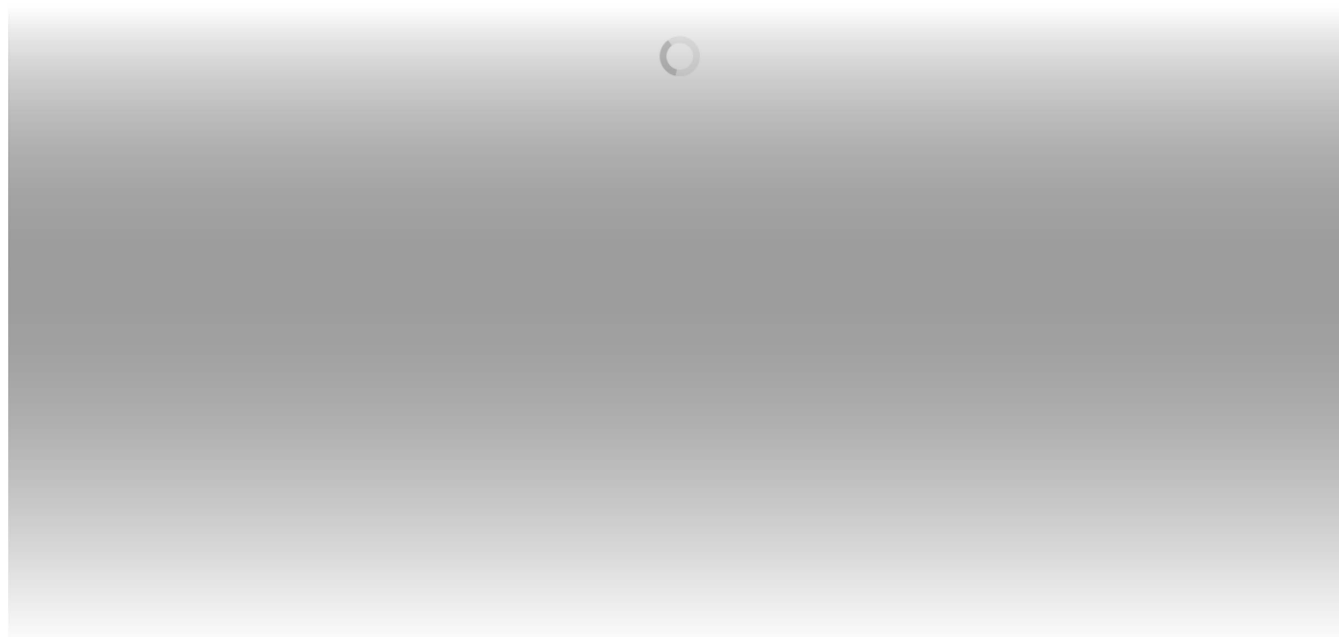
<https://patentscope.wipo.int/search/en/result.jsf?inchikey=OWQCHLFKOGVODW-UHFFFAOYSA-M>

▶ PATENTSCOPE (WIPO)

9 Classification



9.1 MeSH Tree



▶ Medical Subject Headings (MeSH)

9.2 NORMAN Suspect List Exchange Classification



▶ NORMAN Suspect List Exchange

9.3 EPA DSSTox Classification



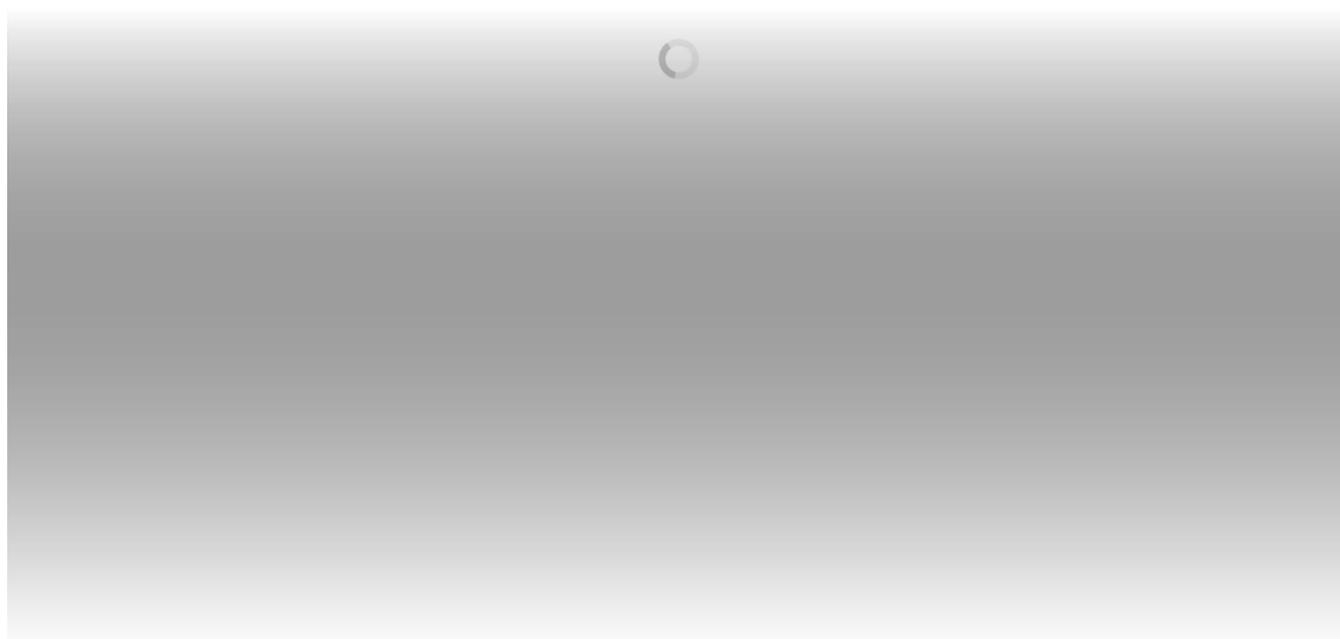
▶ EPA DSSTox

9.4 PFAS and Fluorinated Organic Compounds in PubChem



▶ PubChem

9.5 EPA Substance Registry Services Tree



▶ EPA Substance Registry Services

10 Information Sources



FILTER BY SOURCE

ALL SOURCES



1. EPA DSSTox

LICENSE

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

Potassium 9-chlorohexadecafluoro-3-oxanonane-1-sulfonate

<https://comptox.epa.gov/dashboard/DTXSID60881236>

CompTox Chemicals Dashboard Chemical Lists

<https://comptox.epa.gov/dashboard/chemical-lists/>

2. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J2.130.971K

3. NORMAN Suspect List Exchange

LICENSE

Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.0

<https://creativecommons.org/licenses/by/4.0/>

Ethanesulfonic acid, 2-[(6-chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl)oxy]-1,1,2,2-tetrafluoro-, potassium salt (1:1)

NORMAN Suspect List Exchange Classification

<https://www.norman-network.com/nds/SLE/>

4. Springer Nature

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=31063313-333708632>

5. PubChem

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

PFAS and Fluorinated Compounds in PubChem

https://gitlab.lcsb.uni.lu/eci/pubchem-docs/-/raw/main/pfas-tree/PFAS_Tree.pdf?inline=false

6. Medical Subject Headings (MeSH)

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<https://www.nlm.nih.gov/copyright.html>

potassium 9-chlorohexadecafluoro-3-oxanonane-1-sulfonate

<https://www.ncbi.nlm.nih.gov/mesh/2101311>

MeSH Tree

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

7. EPA Substance Registry Services

LICENSE

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

EPA SRS List Classification

https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

8. PATENTSCOPE (WIPO)

SID 469697708

<https://pubchem.ncbi.nlm.nih.gov/substance/469697708>

