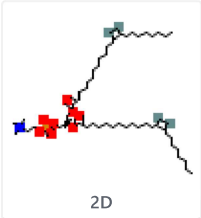
PubChem

COMPOUND SUMMARY

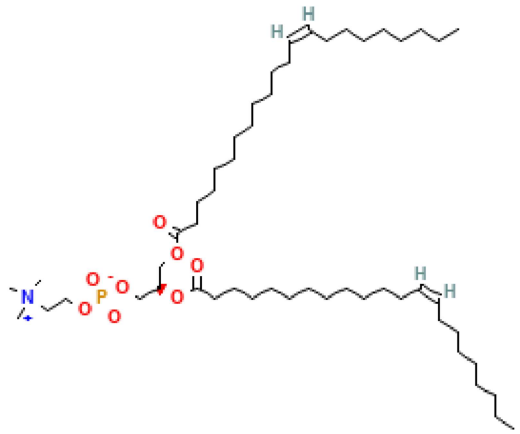
1,2-Dierucoyl-sn-glycero-3-phosphocholine

PubChem CID	24779126
Structure	 2D Find Similar Structures
Molecular Formula	$C_{52}H_{100}NO_8P$
Synonyms	1,2-Dierucoyl-sn-glycero-3-phosphocholine 51779-95-4 L-Dierucoyl lecithin Dierucoyllecithin DEPC, L- More...
Molecular Weight	898.3
Parent Compound	 CID 5313689 (Dierucoylphosphatidylcholine)
Dates	Modify 2023-03-11 Create 2008-05-14

1 Structures

1.1 2D Structure

Chemical Structure Depiction



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1.2 3D Status

Conformer generation is disallowed since too many atoms, too flexible

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2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

[(2*R*)-2,3-bis[[(*Z*)-docos-13-enoyl]oxy]propyl] 2-(trimethylazaniumyl)ethyl phosphate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

2.1.2 InChI

InChI=1S/C52H100NO8P/c1-6-8-10-12-14-16-18-20-22-24-26-28-30-32-34-36-38-40-42-44-51(54)58-48-50(49-60-62(56,57)59-47-46-53(3,4)5)61-52(55)45-43-41-39-37-35-33-31-29-27-25-23-21-19-17-15-13-11-9-7-2/h20-23,50H,6-19,24-49H2,1-5H3/b22-20-,23-21-/t50-/m1/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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2.1.3 InChIKey

SDEURMLKLAEUAY-JFSPZUDSSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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2.1.4 Canonical SMILES

CCCCCCCCC=CCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCC=CCCCCCCCC

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.1.5 Isomeric SMILES

CCCCCCCC/C=C\CCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCC/C=C\CCCCCCCC

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.2 Molecular Formula

C52H100NO8P

Computed by PubChem 2.1 (PubChem release 2021.05.07)

PubChem

2.3 Other Identifiers

2.3.1 CAS

51779-95-4

ChemIDplus; EPA DSSTox; FDA Global Substance Registration System (GSRS)

76420-81-0

ChemIDplus

2.3.2 UNII

1Z951826B6

FDA Global Substance Registration System (GSRS)

2.3.3 DSSTox Substance ID

DTXSID401345798

EPA DSSTox

2.3.4 Wikidata

Q27253299

Wikidata

2.3.5 Metabolomics Workbench ID

13662

Metabolomics Workbench

2.4 Synonyms

2.4.1 MeSH Entry Terms

1,2-didocos-13-enoyl phoshatidylcholine

Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

1,2-Dierucoyl-sn-glycero-3-phosphocholine
51779-95-4
L-Dierucoyl lecithin
Dierucoyllecithin
DEPC, L-
DEPC, R-
1,2-DI13-CIS-DOCOSENOYL-SN-GLYCERO-3-PHOSPHOCHOLINE
1,2-Dierucoyl-phosphatidylcholine, r-
1,2-Dierucoyl-sn-glycerol-3-phosphorylcholine
PC(22:1/22:1)
Dierucoyl-L-a-glycerophosphorylcholine
1,2-di-(13Z-docosenoyl)-sn-glycero-3-phosphocholine
PC(22:1(13Z)/22:1(13Z))
1Z951826B6
1,2-Dierucoyl-sn-Glycero-3-Phosphatidylcholine
[(2R)-2,3-bis[[(Z)-docos-13-enoyl]oxy]propyl] 2-(trimethylazaniumyl)eth
3,5,9-Trioxa-4-phosphahentriacont-22-en-1-aminium, 4-hydroxy-N,N,N-salt, 4-oxide, (7R,22Z)-
Dierucoylphosphatidylcholine
3,5,9-Trioxa-4-phosphahentriacont-22-en-1-aminium, 4-hydroxy-N,N,N-salt, 4-oxide, (7R,22Z)-
UNII-1Z951826B6
Dierucoyl phosphatidylcholine
SCHEMBL178155

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3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	898.3	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	18.1	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	8	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	50	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	897.71865615	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	897.71865615	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	111 Å^2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	62	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	1100	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	1	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	2	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

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3.2 Experimental Properties

3.2.1 Physical Description

Solid

Human Metabolome Database (HMDB)

4 Spectral Information

4.1 Mass Spectrometry

4.1.1 MS-MS

Showing 2 of 4 View More

Spectra ID	2240840
Ionization Mode	Positive
SPLASH	splash10-002r-8900000000-64aed60867a48c13dadf
Top 5 Peaks	86.09728 100 125.0011 81.55 184.07487 46.57 98.9848 15.41 71.07373 13.72
Thumbnail	

Human Metabolome Database (HMDB)

Spectra ID	2240868
Ionization Mode	Positive
SPLASH	splash10-002r-8900000000-27dcd0bb84279f3cde72
Top 5 Peaks	86.0973 100 125.00116 80.14 184.07496 44.69 98.98482 17.26 71.07376 13.21
Thumbnail	

Human Metabolome Database (HMDB)

4.1.2 LC-MS

Showing 2 of 3 View More

MoNA ID	EMBL-MCF_spec339300
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M+H]+
Precursor m/z	898.728186939542
Instrument	Thermo Q-Exactive Plus
Instrument Type	LC-ESI-QFT
Ionization Mode	positive
Collision Energy	60.0 eV
Top 5 Peaks	86.0972813296 100 125.001095587 81.55 184.074872258 46.57 98.9847959018 15.41 71.0737319847 13.72
SPLASH	splash10-002r-8900000000-7e389036244f48378aaf
Thumbnail	
Submitter	Prasad Phapale, EMBL - Metabolomics Core Facility

MassBank of North America (MoNA)

MoNA ID	EMBL-MCF_spec339303
MS Category	Experimental
MS Type	LC-MS

MS Level	MS2
Precursor Type	[M+H]+
Precursor m/z	898.729709916984
Instrument	Thermo Q-Exactive Plus
Instrument Type	LC-ESI-QFT
Ionization Mode	positive
Collision Energy	60.0 eV
Top 5 Peaks	86.0972775625 100 125.001090901 80.41 184.074843187 46.31 98.9847803108 17.55 71.0737441897 12.94
SPLASH	splash10-002r-8900000000-69194839e7805f725231
Thumbnail	
Submitter	Prasad Phapale, EMBL - Metabolomics Core Facility

▸ MassBank of North America (MoNA)

4.1.3 Other MS

MoNA ID	CCMSLIB00000479567
MS Category	Experimental
MS Level	MS2
Precursor Type	[M+H]+
Precursor m/z	898.33
Instrument	Q-Exactive Plus
Ionization Mode	positive
Top 5 Peaks	184.083572 100 86.098190 5.57 125.004265 2.28 104.109001 0.90 71.073753 0.31
SPLASH	splash10-001i-0900000000-a332be042094a5f18fdc
Thumbnail	

Submitter	GNPS Team, University of California, San Diego

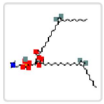
MassBank of North America (MoNA)

5 Related Records

5.1 Related Compounds with Annotation

PubChem

5.2 Parent Compound



CID 5313689 (Dierucoylphosphatidylcholine)

PubChem

5.3 Related Compounds

Same Connectivity	6 Records
Same Parent, Connectivity	12 Records
Same Parent, Exact	2 Records
Mixtures, Components, and Neutralized Forms	1 Record
Similar Compounds	5,107 Records

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5.4 Substances

5.4.1 Related Substances

Same	52 Records

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5.4.2 Substances by Category