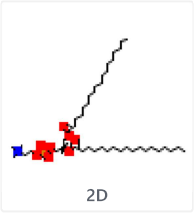
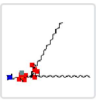
PubChem

COMPOUND SUMMARY

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

PubChem CID	94190
Structure	 2D Find Similar Structures
Molecular Formula	$C_{44}H_{88}NO_8P$
Synonyms	1,2-Distearoyl-sn-glycero-3-phosphocholine 816-94-4 DSPC Distearoyl phosphatidylcholine (R)-2,3-Bis(stearoyloxy)propyl (2-(trimethylammonio)ethyl) phosphate More...
Molecular Weight	790.1
Parent Compound	 CID 94191 (DI-Stearoyl-3-SN-phosphatidylcholine)
Dates	Modify 2023-03-11 Create 2005-03-26

1,2-distearoyl-sn-glycero-3-phosphocholine is a phosphatidylcholine 36:0 in which both phosphatidyl acyl groups are specified as stearoyl (octadecanoyl). It is functionally related to an octadecanoic acid.

▶ ChEBI

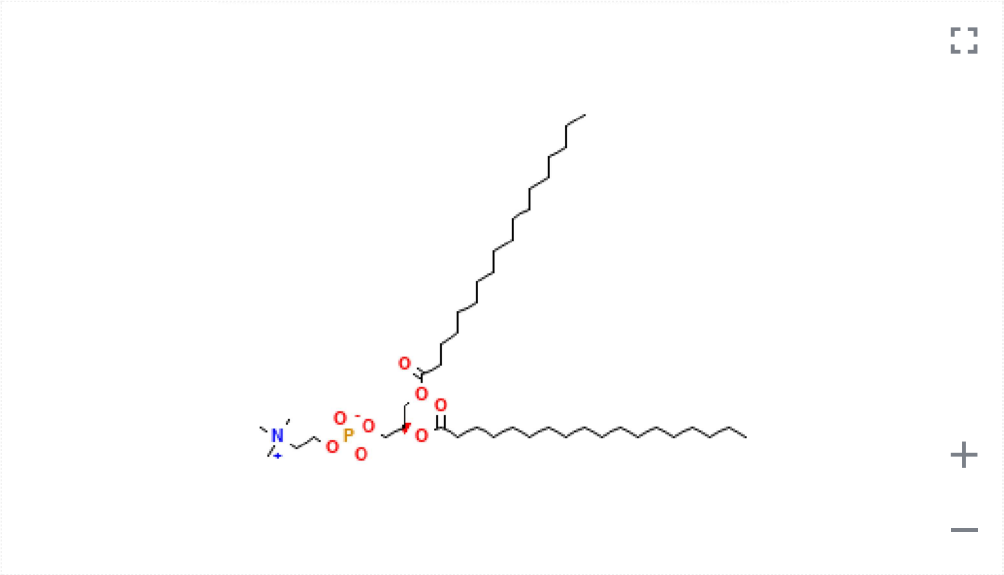
PC(18:0/18:0) is a metabolite found in or produced by Saccharomyces cerevisiae.

▶ Yeast Metabolome Database (YMDB)

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-di(octadecanoyloxy)propyl] 2-(trimethylazaniumyl)ethyl phosphate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

2.1.2 InChI

InChI=1S/C44H88NO8P/c1-6-8-10-12-14-16-18-20-22-24-26-28-30-32-34-36-43(46)50-40-42(41-52-54(48,49)51-39-38-45(3,4)5)53-44(47)37-35-33-31-29-27-25-23-21-19-17-15-13-11-9-7-2/h42H,6-41H2,1-5H3/t42-/m1/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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2.1.3 InChIKey

NRJAVPSFFCBXDT-HUESYALOSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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2.1.4 Canonical SMILES

CCCCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCCCCC

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.1.5 Isomeric SMILES

CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCCCCC

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.2 Molecular Formula

C44H88NO8P

Computed by PubChem 2.1 (PubChem release 2021.05.07)

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2.3 Other Identifiers

2.3.1 CAS

816-94-4

CAS Common Chemistry; ChemIDplus; DTP/NCI; EPA DSSTox; European Chemicals Agency (ECHA); FDA Global Substance Registration System (GSRS)

2.3.2 European Community (EC) Number

212-440-2

European Chemicals Agency (ECHA)

2.3.3 NSC Number

725285

DTP/NCI

2.3.4 UNII

043IPI2M0K

FDA Global Substance Registration System (GSRS)

2.3.5 DSSTox Substance ID

DTXSID20231218

EPA DSSTox

2.3.6 Wikipedia

Distearoylphosphatidylcholine

Wikipedia

2.3.7 Wikidata

Q27157143

Wikidata

2.3.8 RXCUI

1426933

NLM RxNorm Terminology

2.3.9 Metabolomics Workbench ID

13299

Metabolomics Workbench

2.4 Synonyms

2.4.1 MeSH Entry Terms

1,2-distearin sn-3-phosphorylcholine	distearoy
1,2-distearoyl-sn-glycero-3-phosphocholine	DL-DSPC
1,2-distearoyllecithin	DSPC R-
1,2-distearoyllecithin, (+-)-isomer	L-distear
1,2-distearoyllecithin, (R)-isomer	L-DSPC
1,2-distearoyllecithin, (S)-isomer	
1,2-distearoylphosphatidylcholine	

4-hydroxy-N,N,N-trimethyl-10-oxo-7-((1-oxooctadecyl)oxy)-3,5,9-trioxa-4-phosphahepta cosan-1-aminium hydroxide, inner salt, 4-oxide
distearoyl phosphatidylcholine
distearoyl-sn-glycero-3-phosphocholine
distearoylglycerophosphocholine

Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

1,2-Distearoyl-sn-glycero-3-phosphocholine	Phosphatidylcholine(18:0/18:0)
816-94-4	GPCho(18:0/18:0)
DSPC	[(2R)-2,3-di(octadecanoyloxy)propyl] 2-(trimethylazaniumyl)ethyl phos
Distearoyl phosphatidylcholine	NSC-725285
(R)-2,3-Bis(stearoyloxy)propyl (2-(trimethylammonio)ethyl) phosphate	UNII-043IPI2M0K
PC(18:0/18:0)	(R)-2,3-Bis(stearoyloxy)propyl [2-(Trimethylammonio)ethyl] Phosphate
1,2-Distearoyl-sn-3-phosphacholine	EINECS 212-440-2
1,2-dioctadecanoyl-sn-glycero-3-phosphocholine	L-beta,gamma,Disteroyl-alpha-lecithin
1,2-distearoyl-sn-glycero-3-phosphorylcholine	MFCD00036905
3-sn-Phosphatidylcholine	L-alpha-Phosphatidylcholine, distearoyl
Di-stearoyl-phosphatidylcholine	1,2-Distearoyl-sn-glycerophosphocholine
043IPI2M0K	DSPC R-ISOMER

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3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	790.1	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	15.6	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	44	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	789.62475576	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	789.62475576	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	54	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	888	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	0	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)

3.2.2 Collision Cross Section

294.94 Å^2 $[M+H]^+$ [CCS Type: DT; Buffer gas: N2; Sample Type: Human plasma; Dataset: Unambiguous Lipids]

DOI:10.1021/acs.jproteome.1c00820

Baker Lab, Chemistry Department, The University of North Carolina at Chapel Hill

3.2.3 Chemical Classes

Lipids -> Unambiguous Lipids

DOI:10.1021/acs.jproteome.1c00820

Baker Lab, Chemistry Department, The University of North Carolina at Chapel Hill

4 Spectral Information

4.1 Mass Spectrometry

4.1.1 MS-MS

Showing 2 of 7 View More

Spectra ID	1472802
Instrument Type	Orbitrap
Ionization Mode	negative
SPLASH	splash10-0089-0000000590-0aad18afe34a7c3e4d4c
Top 5 Peaks	834.6193 62.65 774.5981 35.64 105.0187 1.70
Thumbnail	
Notes	adduct_type [M+HCO2]- original_collision_energy 20 nominal CannabisDB spectra from NIST14 2020 June Thermo Finnigan Elite Orbitrap

Human Metabolome Database (HMDB)

Spectra ID	1472803
Instrument Type	Orbitrap
Ionization Mode	negative
SPLASH	splash10-00e9-0000000950-0e01653ba450f4cf2474
Top 5 Peaks	774.5991 61.61 834.6193 35.35 283.2629 3.04
Thumbnail	

Notes	adduct_type [M+HCO2]- original_collision_energy 25 nominal CannabisDB spectra from NIST14 2020 June Thermo Finnigan Elite Orbitrap

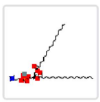
▸ Human Metabolome Database (HMDB)

5 Related Records

5.1 Related Compounds with Annotation

PubChem

5.2 Parent Compound



CID 94191 (DI-Stearoyl-3-SN-phosphatidylcholine)

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5.3 Related Compounds

Same Connectivity	12 Records
Same Stereo	9 Records
Same Isotope	3 Records
Same Parent, Connectivity	44 Records
Same Parent, Stereo	26 Records
Same Parent, Isotope	24 Records
Same Parent, Exact	9 Records
Mixtures, Components, and Neutralized Forms	1 Record
Similar Compounds	1,535 Records

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5.4 Substances

5.4.1 Related Substances

Same	89 Records

PubChem

5.4.2 Substances by Category

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5.5 Entrez Crosslinks

PubMed	2 Records

PubChem