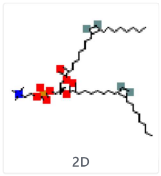
PubChem

COMPOUND SUMMARY

1,2-Dioleoyl-sn-Glycero-3-Phosphocholine

PubChem CID	10350317
Structure	 2D Find Similar Structures
Molecular Formula	$C_{44}H_{84}NO_8P$
Synonyms	1,2-Dioleoyl-sn-Glycero-3-Phosphocholine 4235-95-4 DOPC PC(18:1(9Z)/18:1(9Z)) 1,2-Dioleoyl-L-alpha-lecithin More...
Molecular Weight	786.1
Parent Compound	 CID 448653
Dates	Modify 2023-03-11 Create 2006-10-25

1,2-dioleoyl-sn-glycero-3-phosphocholine is a phosphatidylcholine 36:2 in which the phosphatidyl acyl groups at positions 1 and 2 are both oleoyl. It is a 1-acyl-2-oleoyl-sn-glycero-3-phosphocholine betaine and a 1,2-di-octadecenoyl-sn-glycero-3-phosphocholine. It is functionally related to an oleic acid. It is a conjugate base of a 1,2-dioleoyl-sn-glycero-3-phosphocholine(1+).

- ChEBI

1,2-Dioleoyl-sn-Glycero-3-Phosphocholine is a natural product found in Trypanosoma brucei with data available.

- LOTUS - the natural products occurrence database

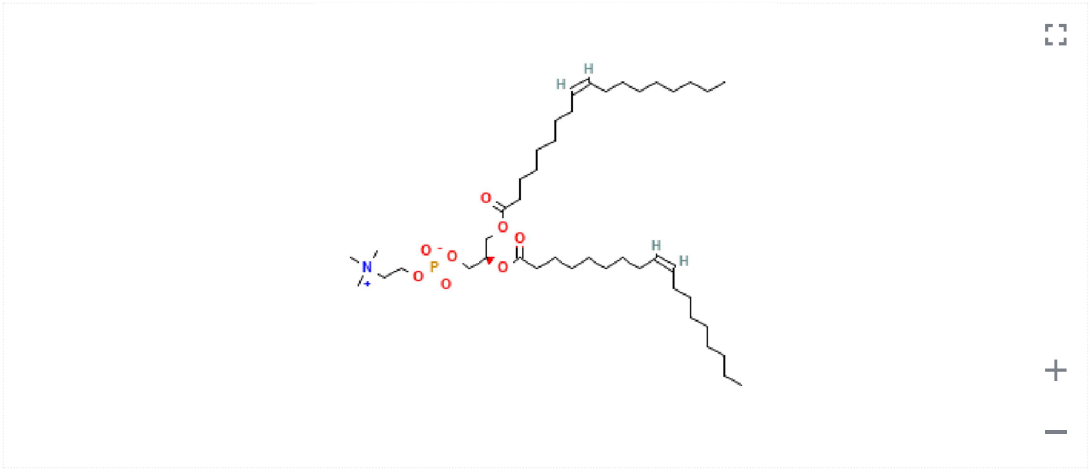
PC(18:1(9Z)/18:1(9Z)) is a metabolite found in or produced by Saccharomyces cerevisiae.

- Yeast Metabolome Database (YMDB)

1 Structures

1.1 2D Structure

Chemical Structure Depiction



PubChem

1.2 3D Status

Conformer generation is disallowed since too many atoms, too flexible

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

[(2*R*)-2,3-bis[[(*Z*)-octadec-9-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/C44H84NO8P/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/h20-23,42H,6-19,24-41H2,1-5H3/b22-20-,23-21-/t42-/m1/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

2.1.3 InChIKey

SNKAWJBJQDLSFF-NVKMUCNASA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

2.1.4 Canonical SMILES

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

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.1.5 Isomeric SMILES

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

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.2 Molecular Formula

C44H84NO8P

Computed by PubChem 2.1 (PubChem release 2021.05.07)

PubChem

2.3 Other Identifiers

2.3.1 CAS

4235-95-4

CAS Common Chemistry; ChemIDplus; EPA DSSTox; European Chemicals Agency (ECHA); FDA Global Substance Registration System (GSRS); Human Metabolome Database (HMDB)

2.3.2 European Community (EC) Number

224-193-8

European Chemicals Agency (ECHA)

2.3.3 UNII

H026DM5V6U

FDA Global Substance Registration System (GSRS)

2.3.4 DSSTox Substance ID

DTXSID101274283

EPA DSSTox

2.3.5 Wikidata

Q27144815

Wikidata

2.3.6 Metabolomics Workbench ID

13545

Metabolomics Workbench

2.4 Synonyms

2.4.1 MeSH Entry Terms

1,2-dioleoyl glycerophosphocholine
1,2-dioleoyl-sn-glycero-3-phosphocholine
1,2-dioleoyl-sn-glycerol-3-ethylphosphocholine
1,2-dioleoylglycerophosphocholine
1,2-DOCPC
1,2-oleoyl-sn-glycero-3-phosphocholine
1,2-oleoylphosphatidylcholine
1,2-oleoylphosphatidylcholine, (E,E)-isomer
1,2-oleoylphosphatidylcholine, (L-alpha)-(R-(Z,Z))-isomer
1,2-oleoylphosphatidylcholine, (R-(E,E))-isomer
1,2-oleoylphosphatidylcholine, (Z,Z)-(+-)-isomer
1,2-oleoylphosphatidylcholine, 14C-labeled, (R-(Z,Z))-isomer
dielaidinoyl lecithin
dielaidoylphosphatidylcholine
dioleoyl lecithin
dioleoyl phosphatidylcholine
dioleoylphosphatidylcholine
dioleoylphosphatidylcholine, DL-
dioleylphosphatidylcholine
DOPC

Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

1,2-Dioleoyl-sn-Glycero-3-Phosphocholine
4235-95-4
DOPC
PC(18:1(9Z)/18:1(9Z))
1,2-Dioleoyl-L-alpha-lecithin
(R)-2,3-Bis(oleoyloxy)propyl (2-(trimethylammonio)ethyl) phosphate
1,2-di-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine
H026DM5V6U
PC(18:1/18:1)
(R)-2,3-Bis(oleoyloxy)propyl [2-(Trimethylammonio)ethyl] Phosphate
Choline phosphate, 3-ester with L-1,2-diolein
(R-(Z,Z))-(7-Oleoyl-4-oxido-10-oxo-3,5,9-trioxa-4-phosphaheptacos-18-enyl)trimethylammonium 4-oxide
Olein, 1,2-di-, L-, dihydrogen phosphate, monoester with choline hydroxic
PC 18:1
PC 36:2
[(2R)-2,3-bis[[(Z)-octadec-9-enoyl]oxy]propyl] 2-(trimethylazaniumyl)ethy
Choline, hydroxide, dihydrogen phosphate, inner salt, ester with L-1,2-dio
dioleoylphosphatidylcholine
UNII-H026DM5V6U
1,2-Dioleoyllec
EINECS 224-193-8
1, 2-dioleoyl-sn-glycero-3-phosphocholine
MFCD00135191
phosphatidylcholine 18:1

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	786.1	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	13.8	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	42	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	785.59345564	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	785.59345564	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	972	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)

PubChem

3.2 Experimental Properties

3.2.1 Physical Description

Solid; [Aldrich MSDS]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Solid

Human Metabolome Database (HMDB)

3.2.2 Collision Cross Section

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

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

298.14 Å^2 [M+CH3COO]$^-$ [CCS Type: DT; Buffer gas: N2; Sample Type: Human bronchoalveolar lavage fluid (BALF); 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

Biological Agents -> Plant Oils and Extracts

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

4 Spectral Information

4.1 Mass Spectrometry

4.1.1 LC-MS

Showing 2 of 3 View More

MoNA ID	HMDB0000593_ms_ms_821
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Instrument Type	Quattro_QQQ
Ionization Mode	positive
Top 5 Peaks	183.0 100 184.0 51.21 85.0 6.64 86.0 4.07 185.0 3.44
SPLASH	splash10-001i-0900000000-ac1e031a7d236f329ed9
Thumbnail	
Submitter	David Wishart, University of Alberta

MassBank of North America (MoNA)

MoNA ID	HMDB0000593_ms_ms_820
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Instrument Type	Quattro_QQQ
Ionization Mode	positive
Top 5 Peaks	183.0 100 184.0 41.91 787.0 6.49 786.0 5.57 185.0 3.33
SPLASH	splash10-001i-0900000000-db47a3894ce23f083a99
Thumbnail	

Submitter	David Wishart, University of Alberta

- MassBank of North America (MoNA)

5 Related Records

5.1 Related Compounds with Annotation

PubChem

5.2 Parent Compound

CID 448653

PubChem

5.3 Related Compounds

Same Connectivity	11 Records
Same Stereo	3 Records
Same Isotope	9 Records
Same Parent, Connectivity	30 Records
Same Parent, Stereo	8 Records
Same Parent, Isotope	25 Records
Same Parent, Exact	3 Records
Mixtures, Components, and Neutralized Forms	1 Record
Similar Compounds	5,107 Records

PubChem

5.4 Substances

5.4.1 Related Substances

Same	76 Records

PubChem

5.4.2 Substances by Category

PubChem

5.5 Entrez Crosslinks

PubMed	2 Records

PubChem

6 Chemical Vendors

- PubChem