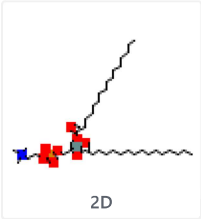
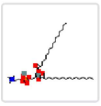
PubChem

COMPOUND SUMMARY

1,2-Dipalmitoylphosphatidylcholine

PubChem CID	6138
Structure	 2D Find Similar Structures
Molecular Formula	$C_{40}H_{80}NO_8P$
Synonyms	2644-64-6 1,2-Dipalmitoyl-rac-glycero-3-phosphocholine 1,2-DIPALMITOYLPHOSPHATIDYLCHOLINE DL-Dipalmitoylphosphatidylcholine DL-beta,gamma-Dipalmitoyl-alpha-lecithin More...
Molecular Weight	734.0
Parent Compound	 CID 6139 (DL-Dipalmitoyllecithin)
Dates	Modify 2023-03-11 Create 2005-08-08

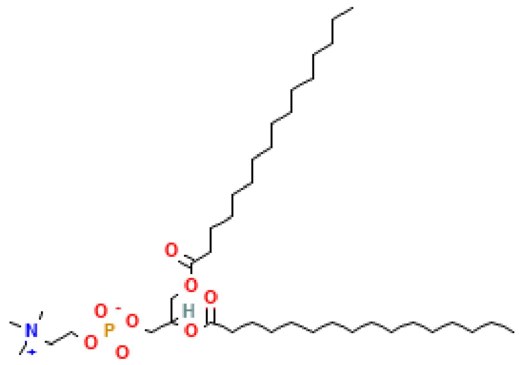
Synthetic phospholipid used in liposomes and lipid bilayers to study biological membranes. It is also a major constituent of PULMONARY SURFACTANTS.

▸ Medical Subject Headings (MeSH)

1 Structures

1.1 2D Structure

Chemical Structure Depiction



PubChem

1.2 3D Status

Conformer generation is disallowed since too flexible

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

2,3-di(hexadecanoyloxy)propyl 2-(trimethylazaniumyl)ethyl phosphate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

2.1.2 InChI

InChI=1S/C40H80NO8P/c1-6-8-10-12-14-16-18-20-22-24-26-28-30-32-39(42)46-36-38(37-48-50(44,45)47-35-34-41(3,4)5)49-40(43)33-31-29-27-25-23-21-19-17-15-13-11-9-7-2/h38H,6-37H2,1-5H3

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

2.1.3 InChIKey

KILNVBDSWZSGLL-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

2.1.4 Canonical SMILES

CCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCCC

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.2 Molecular Formula

C40H80NO8P

Computed by PubChem 2.1 (PubChem release 2021.05.07)

PubChem

2.3 Other Identifiers

2.3.1 CAS

2644-64-6

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

2.3.2 Deprecated CAS

159022-81-8, 173839-68-4, 2797-68-4, 67118-46-1, 36441-53-9, 82623-33-4, 90289-55-7, 107041-15-6, 215369-06-5

ChemIDplus

2.3.3 European Community (EC) Number

220-153-9

- European Chemicals Agency (ECHA)

2.3.4 UNII

2W15RT5V7V

- FDA Global Substance Registration System (GSRS)

2.3.5 DSSTox Substance ID

DTXSID50910226

- EPA DSSTox

2.3.6 Wikipedia

Dipalmitoylphosphatidylcholine

- Wikipedia

2.3.7 Wikidata

Q2587934

- Wikidata

2.3.8 RXCUI

1926947

- NLM RxNorm Terminology

2.4 Synonyms

2.4.1 MeSH Entry Terms

1,2 Dihexadecyl sn Glycerophosphocholine
1,2 Dipalmitoyl Glycerophosphocholine
1,2 Dipalmitoylphosphatidylcholine
1,2-Dihexadecyl-sn-Glycerophosphocholine
1,2-Dipalmitoyl-Glycerophosphocholine
1,2-Dipalmitoylphosphatidylcholine
Dipalmitoyl Phosphatidylcholine
Dipalmitoylglycerophosphocholine
Dipalmitoyllecithin
Dipalmitoylphosphatidylcholine
Phosphatidylcholine, Dipalmitoyl

- Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

2644-64-6	rac-1,2-Dipalmitoylglycerol-3-phosphorylcholine	2
1,2-Dipalmitoyl-rac-glycero-3-phosphocholine	2,3-di(hexadecanoyloxy)propyl 2-(trimethylazaniumyl)ethyl phosphate	3
1,2-DIPALMITOYLPHOSPHATIDYLCHOLINE	Dihexadecanoyl phosphatidylcholine	D
DL-Dipalmitoylphosphatidylcholine	DL-3-Dipalmitoylphosphatidylcholine	L
DL-beta,gamma-Dipalmitoyl-alpha-lecithin	1,2-Dihexadecanoyl phosphatidylcholine	U
2797-68-4	1,2-Dipalmitoylglycerophosphorylcholine	b
1,2-DIHEXADECANOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE	rac-1,2-Dipalmitoylphosphatidylcholine	D
DPPC (phosphatide)	1,2-Dipalmitoyl-3-phosphatidyl choline	1,
1,2-Dipalmitoyl-DL-phosphatidylcholine	dl-1,2-Dipalmitoyl-3-phosphatidylcholine	M
Coatsome MC 6060	1-Palmitoyl-2-palmitoylphosphatidylcholine	E
1,2-Dipalmitoyllecithin	1,2-Dipalmitoylglycerol-3-phosphorylcholine	E
2W15RT5V7V	Choline, phosphate, ester with 1,2-dipalmitin	a

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	734.0	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	13.5	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	40	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	733.56215551	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	733.56215551	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	50	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	826	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	1	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)

PubChem

3.2 Experimental Properties

3.2.1 Physical Description

White powder; [Aldrich MSDS]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

3.2.2 Chemical Classes

Biological Agents -> Plant Oils and Extracts

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

4 Spectral Information

4.1 1D NMR Spectra

4.1.1 13C NMR Spectra

Copyright	Copyright © 2016-2021 W. Robien, Inst. of Org. Chem., Univ. of Vienna. All Rights Reserved.

Thumbnail

SpectraBase

4.2 Mass Spectrometry

4.2.1 GC-MS

Source of Spectrum	EP-4664-0-0
Copyright	Copyright © 2020-2021 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

SpectraBase

Source of Spectrum	JZ-1992-3073-0
Copyright	Copyright © 2020-2021 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail	

SpectraBase

4.2.2 LC-MS

Showing 2 of 19 View More

Accession ID	MSBNK-Chubu_Univ-UT001011
Authors	Taguchi R, Graduate School of Medicine, The University of Tokyo
Instrument	LC-10ADVPmicro HPLC, Shimadzu; LTQ Orbitrap, Thermo Scientific
Instrument Type	LC-ESI-ITFT
MS Level	MS2
Ionization Mode	NEGATIVE
Ionization	ESI
Collision Energy	30%
Column Name	Develosil C30, Nomura Chemical
Retention Time	26.98 min (in paper: 26.9 min)
Precursor m/z	792.57
Precursor Adduct	[M+CH3COO]-
Top 5 Peaks	718.16 999 329.13 8 255.15 8 283.08 8 303.17 3
SPLASH	splash10-014i-0000000900-6acb075cc890d1ad974d
Thumbnail	

License	CC BY-NC-SA
Reference	Taguchi, R.; Ishikawa, M. Precise and Global Identification of Phospholipid Molecular Species by an Orbitrap Mass Spectrometer and Automated Search Engine Lipid Search. Journal of Chromatography A 2010, 1217 (25), 4229–39. DOI:10.1016/j.chroma.2010.04.034

▶ MassBank Europe

Accession ID	MSBNK-Chubu_Univ-UT001287
Authors	Taguchi R, Graduate School of Medicine, The University of Tokyo
Instrument	LC-10ADVPmicro HPLC, Shimadzu; LTQ Orbitrap, Thermo Scientific
Instrument Type	LC-ESI-ITFT
MS Level	MS2
Ionization Mode	NEGATIVE
Ionization	ESI
Collision Energy	30%
Column Name	Develosil C30, Nomura Chemical
Retention Time	27.03 min (in paper: 26.9 min)
Precursor m/z	792.58
Precursor Adduct	[M+CH3COO]-
Top 5 Peaks	718.16 999 255.09 7 733.08 6 718.85 3 480.06 2
SPLASH	splash10-014i-0000000900-ce5ac683049304c15925
Thumbnail	
License	CC BY-NC-SA
Reference	Taguchi, R.; Ishikawa, M. Precise and Global Identification of Phospholipid Molecular Species by an Orbitrap Mass Spectrometer and Automated Search Engine Lipid Search. Journal of Chromatography A 2010, 1217 (25), 4229–39. DOI:10.1016/j.chroma.2010.04.034

▶ MassBank Europe

4.2.3 Other MS

Showing 2 of 4 View More

MoNA ID	LipidBlast2022_454019
MS Category	Experimental
Precursor Type	[M+H]+
Precursor m/z	734.56943
Ionization Mode	positive
Top 5 Peaks	184.0733 100 734.5695 30.03 496.3405 5.01 478.3299 5.01
SPLASH	splash10-001i-0900000200-77f1c042151637394f3b
Thumbnail	
Submitter	Hiroshi Tsugawa, RIKEN

MassBank of North America (MoNA)

MoNA ID	LipidBlast2022_481680
MS Category	Experimental
Precursor Type	[M+Na]+
Precursor m/z	756.55138
Ionization Mode	positive
Top 5 Peaks	756.5514 100 573.4854 60.06 697.4779 50.05 146.9818 40.04 551.5029 40.04
SPLASH	splash10-0aba-0300094800-b2fe3359cb459b2da0c5
Thumbnail	