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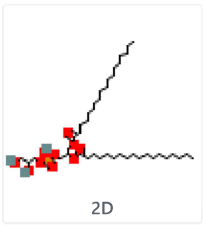
COMPOUND SUMMARY

Distearoyl phosphatidylglycerol

PubChem CID	65145
Structure	 2D Find Similar Structures
Molecular Formula	$C_{42}H_{83}O_{10}P$
Synonyms	Distearoyl ppg DSPG Distearoyl phosphatidylglycerol 4537-78-4 4271ZA8WXO More...
Molecular Weight	779.1
Dates	Modify 2023-03-11 Create 2005-08-08

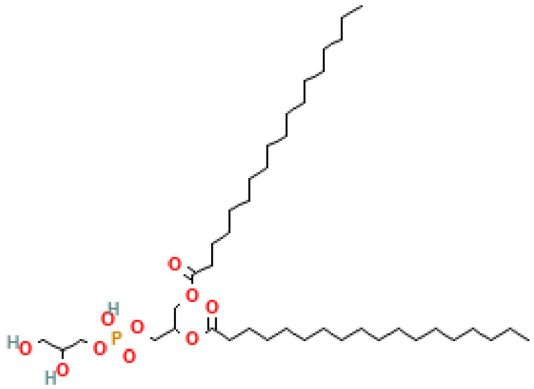
Distearoyl phosphatidylglycerol is a phosphatidylglycerol in which the phosphatidyl acyl groups are both stearoyl.

▸ ChEBI

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

[3-[2,3-dihydroxypropoxy(hydroxy)phosphoryl]oxy-2-octadecanoyloxypropyl] octadecanoate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

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2.1.2 InChI

InChI=1S/C42H83O10P/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-41(45)49-37-40(38-51-53(47,48)50-36-39(44)35-43)52-42(46)34-32-30-28-26-24-22-20-18-16-14-12-10-8-6-4-2/h39-40,43-44H,3-38H2,1-2H3,(H,47,48)

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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2.1.3 InChIKey

FVJZSBGHRPJMMA-UHFFFAOYSA-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(CO)O)OC(=O)CCCCCCCCCCCCCCCCC

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

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2.2 Molecular Formula

C42H83O10P

Computed by PubChem 2.1 (PubChem release 2021.05.07)

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2.3 Other Identifiers

2.3.1 CAS

4537-78-4

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

2.3.2 UNII

4271ZA8WXO

FDA Global Substance Registration System (GSRS)

2.3.3 DSSTox Substance ID

DTXSID30963376

EPA DSSTox

2.3.4 Wikidata

Q27130594

Wikidata

2.3.5 RXCUI

1942751

NLM RxNorm Terminology

2.4 Synonyms

2.4.1 MeSH Entry Terms

1,2-distearoylphosphatidylglycerol
distearoyl phosphatidylglycerol
distearoyl phosphatidylglycerol, sodium
distearoyl PPG
DSPG

Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

Distearoyl ppg	dioctanoylphosphatididylglycerol
DSPG	SCHEMBL21434493
Distearoyl phosphatidylglycerol	CHEBI:61056
4537-78-4	DTXSID30963376
4271ZA8WXO	C18:0 PG
[3-[2,3-dihydroxypropoxy(hydroxy)phosphoryl]oxy-2-octadecanoyloxypropyl] octadecanoate	DSPG, (+/-)-
Octadecanoic acid, 1-((((2,3-dihydroxypropoxy)hydroxyphosphinyl)oxy)methyl)-1,2-ethanediyl ester	DISTEAROYLPHOSPHATIDYLGLYCER(
Distearoylphosphatidylglycerol	1,2-di-O-stearoyl-rac-3-glycerophosp
UNII-4271ZA8WXO	FT-0650998
18:0 PG	1,2-di-O-octadecanoyl-rac-3-glycero
DSPG, DL-	1,2-Distearoyl-sn-glycero-3-phospho
distearoylphoshatidylglycerol	STEARIN, 1,2-DI-, 1-GLYCEROPHOSPH

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3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	779.1	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	14.3	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	10	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	778.57238584	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	778.57238584	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	149 Å^2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	53	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	858	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	2	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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4 Spectral Information

4.1 Mass Spectrometry

4.1.1 LC-MS

MoNA ID	CCMSLIB00005436448
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M-H]-
Precursor m/z	777.565
Instrument	qTof
Ionization Mode	negative
Top 5 Peaks	777.562378 100 283.264252 88.58 778.563660 83.61 742.584167 36.83 779.565552 31.12
SPLASH	splash10-0059-0030000900-2555cea1b2bbf4d030ef
Thumbnail	
Submitter	GNPS Team, University of California, San Diego

▶ MassBank of North America (MoNA)

4.1.2 Other MS

MoNA ID	LipidBlast2022_540492
MS Category	Experimental
Precursor Type	[M+NH4]+
Precursor m/z	796.60621
Ionization Mode	positive
Top 5 Peaks	607.5671 100 341.305 5.01

	796.6062 5.01
SPLASH	splash10-0a4i-0000009000-97ed8382ba1ecc122de4
Thumbnail	
Submitter	Hiroshi Tsugawa, RIKEN

▶ MassBank of North America (MoNA)

MoNA ID	LipidBlast2022_1291915
MS Category	Experimental
Precursor Type	[M-H]-
Precursor m/z	777.56511
Ionization Mode	negative
Top 5 Peaks	283.2635 100 777.5651 50.05 511.3038 20.02 493.2932 20.02
SPLASH	splash10-003r-0090110400-e74fa59d5d918293f3d0
Thumbnail	
Submitter	Hiroshi Tsugawa, RIKEN

▶ MassBank of North America (MoNA)

5 Related Records

5.1 Related Compounds with Annotation

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5.2 Related Compounds

Same Connectivity	6 Records
Same Isotope	5 Records
Same Parent, Connectivity	17 Records
Same Parent, Isotope	15 Records
Same Parent, Exact	4 Records
Mixtures, Components, and Neutralized Forms	5 Records
Similar Compounds	6,426 Records

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5.3 Substances

5.3.1 Related Substances

All	62 Records
Same	28 Records
Mixture	34 Records

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5.3.2 Substances by Category

- PubChem

6 Chemical Vendors

- PubChem