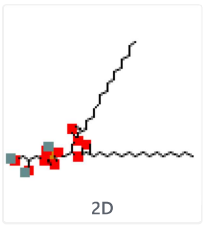
PubChem

COMPOUND SUMMARY

Dipalmitoylphosphatidylglycerol

PubChem CID	65144
Structure	 2D Find Similar Structures
Molecular Formula	$C_{38}H_{75}O_{10}P$
Synonyms	Dipalmitoylphosphatidylglycerol 4537-77-3 DPPG 1,2-Dipalmitoylphosphatidylglycerol VA9U6BR3SB More...
Molecular Weight	723.0
Dates	Modify 2023-03-25 Create 2005-08-08

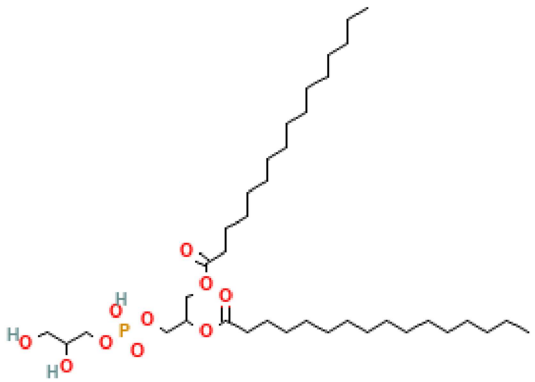
Dipalmitoyl phosphatidylglycerol is a phosphatidylglycerol in which the phosphatidyl acyl groups are both palmitoyl. It is functionally related to a hexadecanoic acid.

▶ ChEBI

1 Structures

1.1 2D Structure

Chemical Structure Depiction



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1.2 3D Status

Conformer generation is disallowed since 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-hexadecanoyloxypropyl] hexadecanoate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

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2.1.2 InChI

InChI=1S/C38H75O10P/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-37(41)45-33-36(34-47-49(43,44)46-32-35(40)31-39)48-38(42)30-28-26-24-22-20-18-16-14-12-10-8-6-4-2/h35-36,39-40H,3-34H2,1-2H3,(H,43,44)

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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2.1.3 InChIKey

BIABMEZBCHDPBV-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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2.1.4 Canonical SMILES

CCCCCCCCCCCCCCCC(=O)OCC(COP(=O)(O)OCC(CO)O)OC(=O)CCCCCCCCCCCCCCC

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

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2.2 Molecular Formula

C38H75O10P

Computed by PubChem 2.1 (PubChem release 2021.05.07)

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2.3 Other Identifiers

2.3.1 CAS

4537-77-3

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

2.3.2 UNII

VA9U6BR3SB

FDA Global Substance Registration System (GSRS)

2.3.3 DSSTox Substance ID

DTXSID70963375

EPA DSSTox

2.3.4 Wikidata

Q27888734

Wikidata

2.3.5 Metabolomics Workbench ID

146654

Metabolomics Workbench

2.4 Synonyms

2.4.1 MeSH Entry Terms

1,2-dipalmitoyl-sn-glycero-3-phosphoglycerol
1,2-dipalmitoylphosphatidylglycerol
dipalmitoylphosphatidylglycerol
DPPG

Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

Dipalmitoylphosphatidylglycerol	starbld0008282
4537-77-3	C16:0 phosphatidylglycerol
DPPG	CHEMBL2286758
1,2-Dipalmitoylphosphatidylglycerol	SCHEMBL13587396
VA9U6BR3SB	DL-dipalmitoylphosphatidylglycerol
CHEBI:60724	DTXSID70963375
[3-[2,3-dihydroxypropoxy(hydroxy)phosphoryl]oxy-2-hexadecanoyloxypropyl] hexadecanoate	C16:0 PG
3-(((2,3-Dihydroxypropoxy)(hydroxy)phosphoryl)oxy)propane-1,2-diyl dipalmitate	DB02043
3-{[(2,3-dihydroxypropoxy)(hydroxy)phosphoryl]oxy}-2-(hexadecanoyloxy)propyl hexadecanoate	DIPALMITOYLPHOSPHATIDYLGLYCERO
1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE	Q27888734
UNII-VA9U6BR3SB	HEXADECANOIC ACID, 1,1'-(1-((((2,3-DI
dipalmitoyl phosphatidylglycerol	Hexadecanoic acid, 1-((((2,3-dihydroxy|

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3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	723.0	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	12.2	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	40	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	722.50978558	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	722.50978558	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	49	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	797	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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3.2 Experimental Properties

3.2.1 Collision Cross Section

263.91 Å^2 [M-H]$^-$ [CCS Type: TW, Method: calibrated with phosphatidylcholines (ESI+) and phosphatidylethanolamines (ESI-) doubly charged cardiolipins calibrated with poly-DL-alanine]

https://www.sciencedirect.com/science/article/pii/S0009308418302238

CCSbase

278.8 Å^2 [M+Na]$^+$ [CCS Type: TW, Method: calibrated with phosphatidylcholines (ESI+) and phosphatidylethanolamines (ESI-) doubly charged cardiolipins calibrated with poly-DL-alanine]

https://www.sciencedirect.com/science/article/pii/S0009308418302238

CCSbase