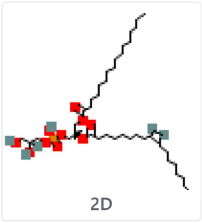
PubChem

COMPOUND SUMMARY

1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphoglycerol

PubChem CID	5283509
Structure	 2D Find Similar Structures
Molecular Formula	$C_{40}H_{77}O_{10}P$
Synonyms	POPG POPG, l- 1-Palmitoyl-2-oleoyl-sn-glycero-3-(phospho-rac-(1-glycerol)) POPG, R- 1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphatidylglycerol More...
Molecular Weight	749.0
Dates	Modify 2023-03-25 Create 2006-01-13

1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoglycerol is a phosphatidylglycerol in which the 1- and 2-acyl groups are specified as palmitoyl and oleoyl respectively. It is functionally related to a hexadecanoic acid and an oleic acid. It is a conjugate acid of a 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoglycerol(1-).

▶ ChEBI

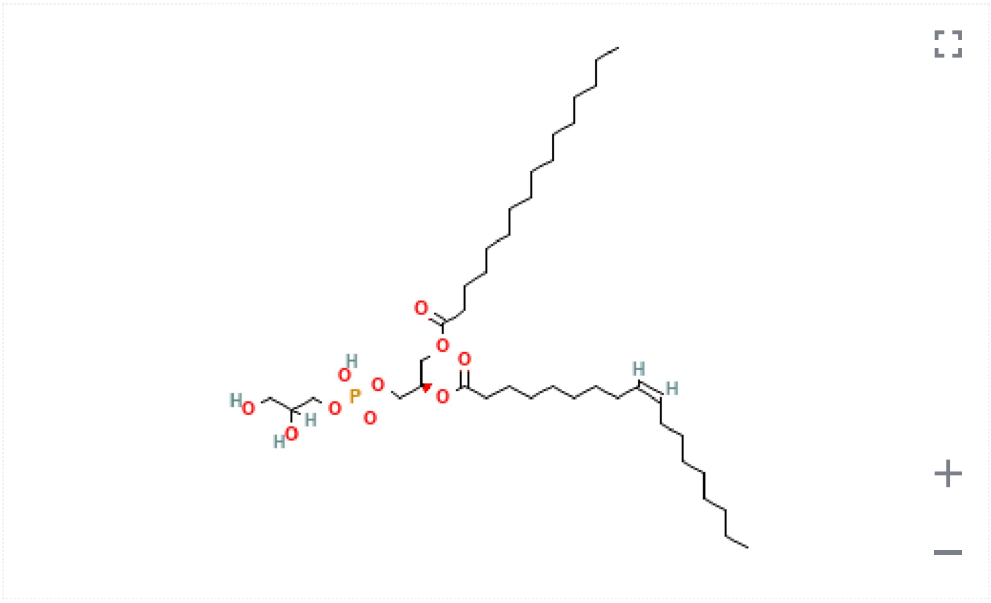
Palmitoyloleoyl-phosphatidylglycerol was a component of Surfaxin, discontinued in 2017, which acted as a surfactant. The product was meant to compensate for alveolar surfactant deficiency and reduce to likelihood of alveolar collapse leading to acute respiratory collapse.

▶ DrugBank

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*)-1-[2,3-dihydroxypropoxy(hydroxy)phosphoryl]oxy-3-hexadecanoyloxypropan-2-yl] (*Z*)-octadec-9-enoate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

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2.1.2 InChI

InChI=1S/C40H77O10P/c1-3-5-7-9-11-13-15-17-18-20-22-24-26-28-30-32-40(44)50-38(36-49-51(45,46)48-34-37(42)33-41)35-47-39(43)31-29-27-25-23-21-19-16-14-12-10-8-6-4-2/h17-18,37-38,41-42H,3-16,19-36H2,1-2H3,(H,45,46)/b18-17-/t37?,38-/m1/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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2.1.3 InChIKey

PAZGBAOHGQRCBP-DDDNOICHSA-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)CCCCCCCC=CCCCCCCCC

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.1.5 Isomeric SMILES

CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)(O)OCC(CO)O)OC(=O)CCCCCCC/C=C\CCCCCCCC

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.2 Molecular Formula

C40H77O10P

Computed by PubChem 2.1 (PubChem release 2021.05.07)

PubChem

2.3 Other Identifiers

2.3.1 CAS

185435-28-3

ChemIDplus; DrugBank; FDA Global Substance Registration System (GSRS)

2.3.2 UNII

F72017VPR7

FDA Global Substance Registration System (GSRS)

2.3.3 Nikkaji Number

J1.014.852I

Japan Chemical Substance Dictionary (Nikkaji)

2.3.4 Wikidata

Q27115796

Wikidata

2.3.5 Metabolomics Workbench ID

152560

Metabolomics Workbench

2.4 Synonyms

2.4.1 Depositor-Supplied Synonyms

POPG	9-Octadecenoic acid (9Z)-
POPG, l-	9-Octadecenoic acid (Z)-,
1-Palmitoyl-2-oleoyl-sn-glycero-3-(phospho-rac-(1-glycerol))	PG(16:0/18:1)
POPG, R-	1-Palmitoyl-2-oleoyl-sn-g
1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphatidylglycerol	UNII-F72017VPR7
185435-28-3	1-Hexadecanoyl-2-(9Z-oc
F72017VPR7	CHEBI:34080
L-alpha-1-Palmitoyl-2-oleoylglycerophosphoglycerol	Palmitoyloleoyl-phosphat
1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphoglycerol	LMGP04010002
1-Palmitoyl-2-oleoyl-sn-glycero-3-phospho-rac-glycerol	1-Palmitoyl-2-oleoyl-sn-g
1-hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycero-3-phospho-(1'-rac-glycerol)	DB11331
[(2R)-1-[2,3-dihydroxypropoxy(hydroxy)phosphoryl]oxy-3-hexadecanoyloxypropan-2-yl] (Z)-octadec-9-enoate	1-Palmitoyl-2-oleoyl-phos

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3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	749.0	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	12.3	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	41	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	748.52543565	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	748.52543565	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	51	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	868	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	1	Computed by PubChem
Defined Bond Stereocenter Count	1	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 MS-MS

NIST Number	1149548
Instrument Type	IT/ion trap
Collision Energy	0
Spectrum Type	MS2
Precursor Type	[M-H]-
Precursor m/z	747.5182
Total Peaks	25
m/z Top Peak	281.2
m/z 2nd Highest	748.5
m/z 3rd Highest	255.2

Thumbnail

NIST Mass Spectrometry Data Center

5 Related Records

5.1 Related Compounds with Annotation

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5.2 Related Compounds

Same Connectivity	16 Records
Same Stereo	3 Records
Same Isotope	14 Records
Same Parent, Connectivity	36 Records
Same Parent, Stereo	10 Records
Same Parent, Isotope	31 Records
Same Parent, Exact	5 Records
Mixtures, Components, and Neutralized Forms	5 Records
Similar Compounds	15,509 Records

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5.3 Substances

5.3.1 Related Substances

All	86 Records
Same	28 Records
Mixture	58 Records

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5.3.2 Substances by Category

- PubChem

6 Chemical Vendors

- PubChem

7 Drug and Medication Information

7.1 Drug Indication

Palmitoyloleoyl-phosphatidylglycerol was a component of Surfaxin which was indicated for the prevention of respiratory distress syndrome in premature infants.

- DrugBank

FDA Label

- DrugBank