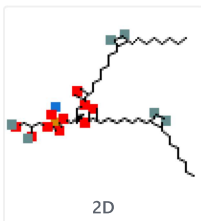





COMPOUND SUMMARY

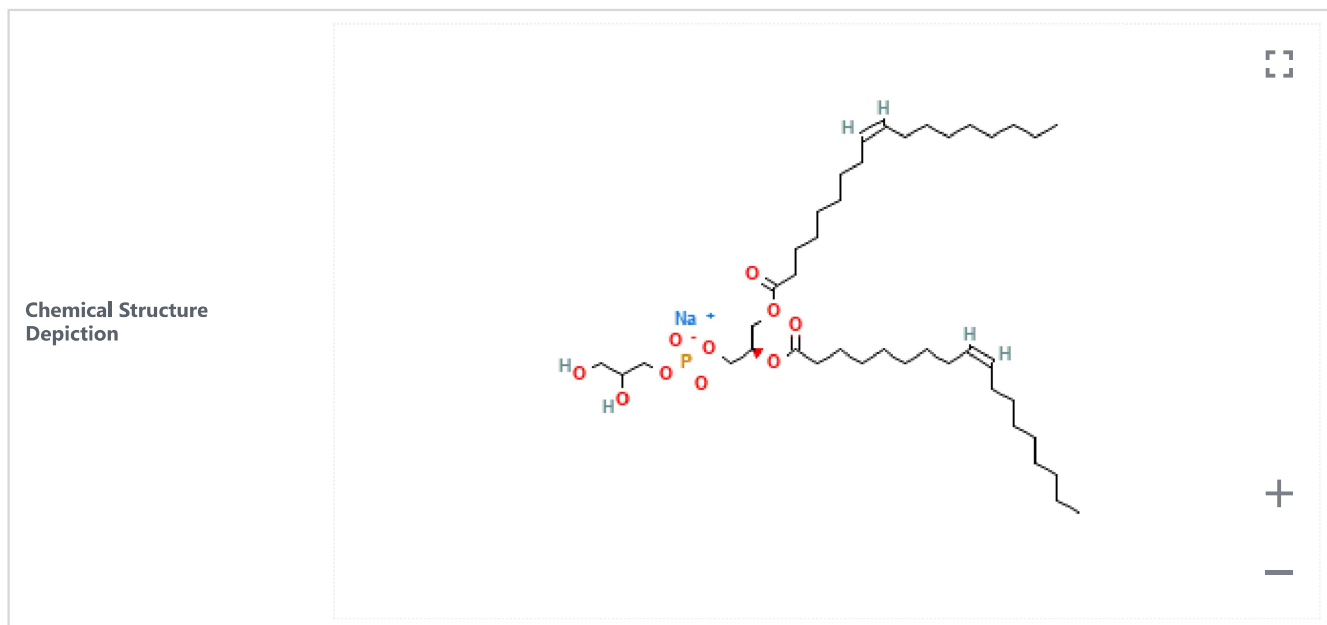
1,2-di-(9Z-octadecenoyl)-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt)

PubChem CID	23702460
Structure	 <p>2D</p> <p>Find Similar Structures</p>
Molecular Formula	$C_{42}H_{78}NaO_{10}P$
Synonyms	<p>67254-28-8 1,2-di-(9Z-octadecenoyl)-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt) DOPG Na, l- DOPG Na, r- DOPG-Na, l-</p> <p>More...</p>
Molecular Weight	797.0
Parent Compound	 <p>CID 11846228 (Dioloylphosphatidylglycerol)</p>
Component Compounds	 <p>CID 5360545 (Sodium)</p>  <p>CID 11846228 (Dioloylphosphatidylglycerol)</p>
Dates	<p>Modify Create</p> <p>2023-03-11 2008-02-05</p>

1 Structures



1.1 2D Structure



► [PubChem](#)

1.2 3D Status



Conformer generation is disallowed since too many atoms, MMFF94s unsupported element, too flexible, mixture or salt

► [PubChem](#)

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



sodium;[(2R)-2,3-bis[[[Z]-octadec-9-enoyl]oxy]propyl] 2,3-dihydroxypropyl phosphate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

[PubChem](#)

2.1.2 InChI



InChI=1S/C42H79O10P.Na/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;/h17-20,39-40,43-44H,3-16,21-38H2,1-2H3,(H,47,48);/q;+1/p-1/b19-17-,20-18-;/t39?,40-;/m1./s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

[PubChem](#)

2.1.3 InChIKey



IUVFCFQZFCOKRC-IPKKNMRRSA-M

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

[PubChem](#)

2.1.4 Canonical SMILES



CCCCCCCC=CCCCCCCC(=O)OCC(COP(=O)([O-])OCC(CO)O)OC(=O)CCCCCCCC=CCCCCCCC.[Na+]

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

[PubChem](#)

2.1.5 Isomeric SMILES



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

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

[PubChem](#)

2.2 Molecular Formula



C42H78NaO10P

Computed by PubChem 2.1 (PubChem release 2021.05.07)

[PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



67254-28-8

2.3.2 UNII



T40U11PG20

▶ FDA Global Substance Registration System (GSRS)

2.3.3 Wikidata



Q27289636

▶ Wikidata

2.4 Synonyms



2.4.1 MeSH Entry Terms



1,2-dioleoyl-sn-glycero-3-phospho(1-rac-glycerol)
1,2-dioleoyl-sn-glycero-3-phosphoglycerol
1,2-dioleoyl-sn-glycero-3-phosphoglycerol, (R-(R*,S*))-(Z)-isomer
1,2-dioleoyl-sn-glycero-3-phosphoglycerol, (Z)-isomer
1,2-dioleoylphosphatidylglycerol
di-C18-1(C)-PG
DOPG

▶ Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms



67254-28-8	sodium
1,2-di-(9Z-octadecenoyl)-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt)	Sodium
DOPG Na, l-	1, 2-dic
DOPG Na, r-	1,2-Dio
DOPG-Na, l-	UNII-T
DOPG-Na, r-	DOPG
T40U11PG20	DOPG-
1,2-Dioleoyl-sn-glycero-3-(phospho-rac-(1-glycerol)), sodium salt	1,2-Dio
1,2-Dioleoyl-sn-glycero-3-phospho-(1'-rac-glycerol), sodium salt	MFCD
sodium;[(2R)-2,3-bis[[[(Z)-octadec-9-enoyl]oxy]propyl] 2,3-dihydroxypropyl phosphate	Dioleo
9-Octadecenoic acid (9Z)-, 1,1'-(1-(((2,3-dihydroxypropoxy)hydroxyphosphinyl)oxy)methyl)-1,2-ethanediyl ester, sodium salt (1:1)	BP-263
1,2-Dioleoyl-sn-glycero-3-phospho(1-rac-glycerol)	D5318

▶ PubChem

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	797.0	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	2	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	42	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	796.52302996	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	796.52302996	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	152 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	948	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	2	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	2	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

► [PubChem](#)

4 Related Records

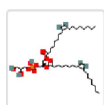


4.1 Related Compounds with Annotation



▶ PubChem

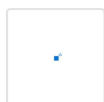
4.2 Parent Compound



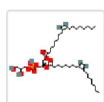
CID 11846228 (Dioleoylphosphatidylglycerol)

▶ PubChem

4.3 Component Compounds



CID 5360545 (Sodium)



CID 11846228 (Dioleoylphosphatidylglycerol)

▶ PubChem

4.4 Related Compounds



Same Connectivity	4 Records
Same Parent, Connectivity	29 Records
Same Parent, Exact	4 Records
Mixtures, Components, and Neutralized Forms	2 Records
Similar Compounds	12,384 Records

▶ PubChem

4.5 Substances



4.5.1 Related Substances



Same	31 Records
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▶ PubChem

4.5.2 Substances by Category



▶ PubChem

▶ PubChem

6 Literature



6.1 NLM Curated PubMed Citations



▶ PubChem

6.2 Springer Nature References



▶ Springer Nature

6.3 General References



Hatzakis et al. How curved membranes recognize amphipathic helices and protein anchoring motifs. *Nature Chemical Biology*, doi: 10.1038/nchembio.213, published online 13 September 2009 <http://www.nature.com/naturechemicalbiology>

▶ [Nature Chemical Biology](#)

Gerlach et al. HIV-1 Nef membrane association depends on charge, curvature, composition and sequence. *Nature Chemical Biology*, doi: 10.1038/nchembio.268, published online 22 November 2009 <http://www.nature.com/naturechemicalbiology>

▶ [Nature Chemical Biology](#)

6.4 Chemical Co-Occurrences in Literature



▶ PubChem

6.5 Chemical-Gene Co-Occurrences in Literature



▶ PubChem

6.6 Chemical-Disease Co-Occurrences in Literature

