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Typical Product Specifications & Properties

1-STEAROYL-2-OLEOYL-SN-GLYCERO-3-[PHOSPHO-L-SERINE](SODIUM SALT)

CAS Number: : 321883-23-2

Specifications	Limits
Chemical Structure	 chemicalStructure-1-stearoyl-2-oleoyl-sn-glycero-3-phospho-l-serine-sodium-salt-
Molecular Formula	C42H79NNaO10P
Molecular weight	
Canonicalized Compound	1
Compound Complexity	986
Hydrogen Bond Acceptor Count	11
Hydrogen Bond Donor Count	2
Rotatable Bond Count	43
Allowed IUPAC Name	sodium;[(2S)-2-amino-2-carboxy-ethyl] [(2R)-3-octadecanoyloxy-2-[(Z)-octadec-9-enoyl]oxy-propyl] phosphate
CAS-like Style IUPAC Name	sodium;[(2S)-2-amino-2-carboxyethyl] [(2R)-2-[(Z)-1-oxooctadec-9-enoxy]-3-(1-oxooctadecoxy)propyl] phosphate
Markup IUPAC Name	sodium;[(2<l>S</l>)-2-amino-2-carboxyethyl] [(2<l>R</l>)-3-octadecanoyloxy-2-[(Z<l>Z</l>)-octadec-9-enoyl]oxypropyl] phosphate
Preferred IUPAC Name	sodium;[(2S)-2-amino-2-carboxyethyl] [(2R)-3-octadecanoyloxy-2-[(Z)-octadec-9-enoyl]oxypropyl] phosphate

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Specifications	Limits
Systematic IUPAC Name	sodium;[(2S)-2-azanyl-3-oxidanyl-3-oxidanylidene-propyl] [(2R)-3-octadecanoyloxy-2-[(Z)-octadec-9-enoyl]oxy-propyl] phosphate
Traditional IUPAC Name	sodium;[(2S)-2-amino-2-carboxy-ethyl] [(2R)-2-[(Z)-octadec-9-enoyl]oxy-3-stearoyloxy-propyl] phosphate
Standard InChI	InChI=1S/C42H80NO10P.Na/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-40(44)50-35-38(36-51-54(48,49)52-37-39(43)42(46)47)53-41(45)34-32-30-28-26-24-22-20-18-16-14-12-10-8-6-4-2;/h18,20,38-39H,3-17,19,21-37,43H2,1-2H3,(H,46,47)(H,48,49);/q;+1/p-1/b20-18-/t38-,39+;/m1./s1
Standard InChIKey	ALPKKMIPHGSQRX-NJZ WBUMZ SA-M
Exact Mass	811.53392900

Specifications Limits

Molecular Weight 812.0

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Canonical SMILES

CCCCCCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC(C(=O)O)N)OC(=O)CCCCCCCC=CCCCCCCCC.
[Na+]

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Monoisotopic Weight

811.53392900



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