

Product Information

2-O-hexadecanoyl-3-O-(2,4S,6S-trimethyl-2E-pentacosenoyl)-6-O-(2,4S,6S-trimethyl-2E-pentacosenoyl)-2'-O-(2R,4S,6S-trimethyl-3R-hydroxy-tetracosanoyl)-4'-O

Cat. No.: X26-02-ZQ5064

Size: 1 mg; 10 mg; 25 mg; 100 mg

Compound CID: 52930179

Synonym:

PAT16(25:1(2E)(2Me,4Me[S],6Me[S])/25:1(2E)(2Me,4Me[S],6Me[S])/24:0(2Me[R],3OH[R],4Me[S],6Me[S])/22:1(2E)(2Me,4Me[S],6Me[S]))

This product is for research use only and is not intended for diagnostic use.

Product Information

Description	Featuring a hydroxylated C24 branch at the 2' position alongside dual C25 branches, this lipid explores site-specific immune recognition. It provides insights into the molecular docking of specialized mycobacterial lipids with host-pattern recognition receptors.
Molecular Weight	2161.5
Molecular Formula	C ₁₃₆ H ₂₅₄ O ₁₇
IUPAC Name	[(3R,5R,6R)-5-hexadecanoyloxy-3-hydroxy-6-[(2R,3S,5S)-4-hydroxy-6-(hydroxymethyl)-3-[(2S,3S,4S,6S)-3-hydroxy-2,4,6-trimethyltetracosanoyl]oxy-5-[(E,4S,6S)-2,4,6-trimethyldocos-2-enoyl]oxyoxan-2-yl]oxy-4-[(E,4S,6S)-2,4,6-trimethylpentacos-2-enoyl]oxyoxan-2-yl)methyl (E,4S,6S)-2,4,6-trimethylpentacos-2-enoate
InChI	InChI=1S/C136H254O17/c1-18-23-28-33-38-43-48-53-57-60-63-67-71-76-80-85-90-95-109(6)100-113(10)104-117(14)131(142)146-108-122-125(140)128(151-133(144)119(16)106-115(12)102-111(8)97-92-87-82-77-72-68-64-61-58-54-49-44-39-34-29-24-19-2)130(149-123(138)99-94-89-84-79-74-65-52-47-42-37-32-27-22-5)136(148-122)153-135-129(152-134(145)120(17)124(139)116(13)103-112(9)98-93-88-83-78-73-69-62-59-55-50-45-40-35-30-25-20-3)126(141)127(121(107-137)147-135)150-132(143)118(15)105-114(11)101-110(7)96-91-86-81-75-70-66-56-51-46-41-36-31-26-21-4/h104-106,109-116,120-122,124-130,135-137,139-141H,18-103,107-108H2,1-17H3/b117-104+,118-105+,119-106+/t109-,110-,111-,112-,113-,114-,115-,116-,120-,121?,122?,124-,125+,126?,127+,128?,129-,130+,135+,136+/m0/s1
InChI Key	IIQNVALLXZTNEY-GDYNOPHQSA-N



Canonical SMILES	<chem>CCCCCCCCCCCCCCCCCCCC[C@H](C)C[C@H](C)/C=C(C)/C(=O)OCC1[C@H](C([C@H]([C@H](O1)O[C@@H]2[C@H](C([C@@H](C(O2)CO)OC(=O)/C=C/[C@@H](C)C[C@@H](C)CCCCCCCCCCCCCCCCC)/C)O)OC(=O)[C@@H](C)[C@H]([C@@H](C)C[C@@H](C)CCCCCCCCCCCCCCCCC)O)OC(=O)CCCCCCCCCCCCCCCC)OC(=O)/C=C/[C@@H](C)C[C@@H](C)CCCCCCCCCCCCCCCCCCCC)/C)O</chem>
Source	Chemical synthesis
Form	Solid or liquid
Purity	≥90%
Identity	Confirmed by NMR/HPLC/MS.
Stability	The product is stable for one year when stored at the recommended temperature in lyophilized powder.
Quality Level	Research level
Applications	Specifically used to study the influence of the 2'-O-hydroxy-C24 chain on the enzymatic degradation of trehalose esters.
Storage	Store at -20°C.
