

Product Name: Thymolphthalexone
Catalog Number: L10962.03

CAS Number: 1913-93-5
IUPAC Name: 2-[[3-[1-(3-[[carboxylatomethyl](carboxymethyl)azaniumyl]methyl)-4-hydroxy-2-methyl-5-(propan-2-yl)phenyl)-3-oxo-1,3-dihydro-2-benzofuran-1-yl]-6-hydroxy-2-methyl-5-(propan-2-yl)phenyl]methyl)(carboxymethyl)azaniumyl]acetate
Molecular Formula: C₃₈H₄₄N₂O₁₂
Molecular Weight: 720.77
MDL Number: MFCD00001619
InChI Key: AGXCADFSYJNMEG-UHFFFAOYNA-N
SMILES: CC(C)C1=CC(=C(C)C(C[NH+](CC(O)=O)CC([O-])=O)=C1O)C1(OC(=O)C2=CC=CC=C12)C1=CC(C(C)C)=C(O)C(C[NH+](CC(O)=O)CC([O-])=O)=C1C
Synonym: 2-[[3-[1-(3-[[carboxylatomethyl](carboxymethyl)ammonio]methyl)-4-hydroxy-5-isopropyl-2-methyl-

Product Specification

Appearance (Color): White to pale brown
Form: powder
Comment: Suitable for use as a complexiometric indicator
Color Change: Blue in alkaline solution
Elemental Analysis: Hydrogen 5.80 - 7.10% (Theory 6.153)
Elemental Analysis: Carbon 64.70-78.40% (Theory 63.323)

Date Of Print: 11/09/2024

Product Specifications are subject to amendment and may change over time. Data contained is accurate as of the date printed.