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Typical Product Specifications & Properties

Thymolphthalexone

CAS Number: : 1913-93-5

Specifications	Limits
Molecular weight	720.77
SMILES	<chem>Cc1c(cc(c(c1C[NH+](CC(=O)O)CC(=O)[O-])O)C(C)C)C2(c3ccccc3C(=O)O2)c4cc(c(c(c4C)C[NH+](CC(=O)O)CC(=O)[O-])O)C(C)C</chem>
InChI	AGXCADFSYJNMEG-UHFFFAOYSA-N
InChIKey	1S/C38H44N2O12/c1-19(2)24-11-29(21(5)26(35(24)49)13-39(15-31(41)42)16-32(43)44)38(28-10-8-7-9-23(28)37(51)52-38)30-12-25(20(3)4)36(50)27(22(30)6)14-40(17-33(45)46)18-34(47)48/h7-12,19-20,49-50H,13-18H2,1-6H3,(H,41,42)(H,43,44)(H,45,46)(H,47,48)
Chemical Structure	 43781_43781_thymolphthalexone.png chemical structure



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