

Typical Product Specifications & Properties

Sodium 4-(3,5,5-Trimethylhexanoyloxy)Benzenesulfonate

CAS Number: : 94612-91-6

Specifications	Limits
SMILES	<chem>[Na+].C(C(C[C@@H](CC(C)(C)C)C)(=O)Oc1ccc(cc1)S(=O)(=O)[O-]</chem>
InChI	GSYPNDDXWAZDJB-UHFFFAOYSA-M
InChIKey	1S/C15H22O5S.Na/c1-11(10-15(2,3)4)9-14(16)20-12-5-7-13(8-6-12)21(17,18)19;/h5-8,11H,9-10H2,1-4H3,(H,17,18,19);/q;+1/p-1