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Typical Product Specifications & Properties

L-Valine Benzyl Ester 4-Toluenesulfonate

CAS Number: : 16652-76-9

Specifications	Limits
Molecular weight	379.47
SMILES	<chem>CC(C)[C@H](N)C(=O)OCc1ccccc1.Cc2ccc(cc2)[S](O)(=O)=O</chem>
InChI	QWUQVUDPBXFOKF-MERQFXBCSA-N
InChIKey	1S/C12H17NO2.C7H8O3S/c1-9(2)11(13)12(14)15-8-10-6-4-3-5-7-10;1-6-2-4-7(5-3-6)11(8,9)10/h3-7,9,11H,8,13H2,1-2H3;2-5H,1H3,(H,8,9,10)/t11-;/m0./s1
Molecular weight	340.41
SMILES	<chem>C(c1ccc(cc1)OCC1CO1)(c1ccc(cc1)OCC1CO1)(C)C</chem>
InChI	1S/C21H24O4/c1-21(2,15-3-7-17(8-4-15)22-11-19-13-24-19)16-5-9-18(10-6-16)23-12-20-14-25-20/h3-10,19-20H,11-14H2,1-2H3
InChIKey	LCFVJGUPQDGYKZ-UHFFFAOYSA-N
Storage Temperature	2-8°C
Water solubility	Soluble in 100% ethanol, dimethyl sulfoxide (100 mM), dimethyl formamide, chloroform, methanol, and ethanol (50 mM). Insoluble in water.
Melting Point	40-44 °C
Refractive Index	1.5735



ISO 9001



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Specifications	Limits
BRN Number	299026
Boiling Point	210 °C / 1mmHg
Density	1,17 g/cm3



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