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Typical Product Specifications & Properties

5-(Methyl-d3)- dibenzothiophenium, 1,1,1- trifluoromethanesulfonate

CAS Number : 2251781-83-4

Specifications	Limits
Chemical Structure	 chemicalStructure-5-methyl-d3-dibenzothiophenium-1-1-1-trifluoromethanesulfonate
Molecular Formula	C14H11F3O3S2
Molecular weight	
Canonicalized Compound	1
Compound Complexity	336
Hydrogen Bond Acceptor Count	6
Hydrogen Bond Donor Count	
Rotatable Bond Count	
Allowed IUPAC Name	5-(trideuteriomethyl)dibenzothiophen-5-ium;trifluoromethanesulfonate
CAS-like Style IUPAC Name	5-(trideuteriomethyl)dibenzothiophen-5-ium;trifluoromethanesulfonate
Markup IUPAC Name	5-(trideuteriomethyl)dibenzothiophen-5-ium;trifluoromethanesulfonate
Preferred IUPAC Name	5-(trideuteriomethyl)dibenzothiophen-5-ium;trifluoromethanesulfonate

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Specifications	Limits
Systematic IUPAC Name	5-(trideuteriomethyl)dibenzothiophen-5-ium;tris (fluoranyl)methanesulfonate
Traditional IUPAC Name	5-(trideuteriomethyl)dibenzothiophen-5-ium;triflate
Standard InChI	InChI=1S/C13H11S.CHF3O3S/c1-14-12-8-4-2-6-10(12)11-7-3-5-9-13(11)14;2-1(3,4)8(5,6)7/h2-9H,1H3;(H,5,6,7)/q+1;/p-1/i1D3;
Standard InChIKey	ROHWBLNJJPWCN-NIIDSAIPSA-M
Exact Mass	351.02900128
Molecular Weight	351.4
Canonical SMILES	<chem>C[S+](C)(C)C1=CC=CC=C2C3=CC=CC=C3C1(C(F)(F)F)S(=O)(=O)[O-]</chem>
Isomeric SMILES	<chem>[2H]C([2H])([2H])C1=CC=CC=C2C3=CC=CC=C3C1(C(F)(F)F)S(=O)(=O)[O-]</chem>
Specifications	Limits
Polar Surface Area	66.6
Topological	
Monoisotopic Weight	351.02900128

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