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Typical Product Specifications & Properties

(E)-4-[3-[2-(trifluoromethyl)-9H-thioxanthen-9-ylidene]propyl]piperazine-1-ethanol

CAS Number: : 53772-85-3

Specifications	Limits
Molecular weight	434.52
EINECS	258-759-0
SMILES	<chem>c1ccc2c(c1)/C(=C\CCN3CCN(CC3)CCO)/c4cc(ccc4S2)C(F)(F)F</chem>
InChI	NJMYODHXAKYRHW-BLLMUTORSA-N
InChIKey	1S/C23H25F3N2OS/c24-23(25,26)17-7-8-22-20(16-17)18(19-4-1-2-6-21(19)30-22)5-3-9-27-10-12-28(13-11-27)14-15-29/h1-2,4-8,16,29H,3,9-15H2/b18-5+
Water solubility	0.346 mg/L
log P (octanol-water)	4.25
Vapor Pressure	1.05E-12 mm Hg
Atmospheric OH Rate Constant	1.71E-10 cm ³ /molecule-sec
Henry's Law Constant	1.6E-16 atm-m ³ /mole



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