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Trifluoromethanesulfinyl Chloride CF₃SOCI

Purity 97%

CAS Number 20621-29-8

Molecular Formula CCIF3OS

Molecular Weight 152.52

Thiotrifluoromethylation, which has excellent lipophilicity, is expected to have unexplored pharmacological effects in pharmaceuticals and agricultural chemicals. Compared to thiotrifluoromethylation of indole with CF3SO2Na, heavy metal reagents such as CuCl are unnecessary, realizing a homogeneous reaction system. Compared to> N-SCF3 series thiotrifluoromethylating agents, it has the advantage of not requiring expensive CF3SAg or CF3Si(Me)3 during reagent preparation.

Application

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No.	CF ₃ SOCI	Solvent	Reductant 1.5 eq	1/2	(%)
#1	1.5 eq	MeCN	PPh3	86/5	
#2	3.0 eq	MeCN	-	83/8	
#3	1.5 eq	MeCN	HP(O)(OEt)2	36/9	

Reaction condition; indole(0.2mmol), Solvent 1ml, under N2, 90degC for 6hr Notes:

Chemistry-A European J. 2018, Vol.24, Issue 70, p18749-18756 Organic & Biomolecular Chemistry, 2016, 14, p7150-7182

Properties:

Appearance Liquid Boiling point, °C 42-43 Flash point, °C -

Capacity: -

Packing: - UN, PG: -