



<chem>COP(=O)(F)CCCC</chem> 		<b>1-METHYLBUTYL METHYLPHOSPHONOFUORIDATE</b>	
CAS number :	761-93-3	Reference :	TMS/internal
MF :	C <sub>6</sub> H <sub>14</sub> FO <sub>2</sub> P	Spectral width :	7692.31 Hz
Solvent/Lock :	CDCl <sub>3</sub> /CDCl <sub>3</sub>	Pulse Width :	5 μs (90°)
Nucleus :	<sup>13</sup> C	Repetition Time :	4 s
Apparatus :	Bruker WP200SY	Data points	FID = 16K, SPC = 8K
Frequency :	50.3 MHz	Line Broadning :	No
Temperature :	23°C	Resolution (TMS) :	1.8 Hz
Concentration :	≈ 40 mg/ml		
		2 Diastereoisomers a : δ <sub>1</sub> = 10.32 ppm ; J <sub>P-a</sub> = 149.3 Hz ; J <sub>F-a</sub> = 28.2 Hz δ <sub>2</sub> = 10.28 ppm ; J <sub>P-a</sub> = 150.2 Hz ; J <sub>F-a</sub> = 28.2 Hz b : δ <sub>1</sub> = 76.24 ppm ; δ <sub>2</sub> = 76.00 ppm ; J <sub>P-b</sub> = 7.5 Hz c : δ = 39.7 ppm ; J <sub>P-c</sub> = 4.7 Hz d : δ <sub>1</sub> = 18.62 ppm ; δ <sub>2</sub> = 18.47 ppm c : δ = 13.73 ppm f : δ <sub>1</sub> = 22.00 ppm ; δ <sub>2</sub> = 21.96 ppm	

OPCW Code:1-3-27 (p1/1)