



>>Entry Name: 2-Chloro-4,4,4-trifluoro-3-oxobutanoic acid, 9Cl

Synonym(s): 2-Chloro-4,4,4-trifluoroacetoacetic acid, 8Cl

$\text{F}_3\text{CCOCHClCOOH}$

Molecular Formula: $\text{C}_4\text{H}_2\text{ClF}_3\text{O}_3$

Molecular Weight: 190.506

Accurate Mass: 189.964456

Percentage Composition: C 25.22%; H 1.06%; Cl 18.61%; F 29.92%; O 25.20%

>>Derivative: Et ester

CAS Registry Number: 363-58-6

Molecular Formula: $\text{C}_6\text{H}_6\text{ClF}_3\text{O}_3$

Molecular Weight: 218.559

Accurate Mass: 217.995756

Percentage Composition: C 32.97%; H 2.77%; Cl 16.22%; F 26.08%; O 21.96%

Physical Description: Liq.

Boiling Point: Bp_{35} 67-71°

Refractive Index: n_D^{23} 1.3880

References:

Walborsky, H.M. *et al.*, *J.A.C.S.*, 1958, **80**, 187, (*Et ester*)