



>>Entry Name: 1,3-Dichloro-1,1,3,3-tetrafluoro-2-propanone, 9CI

Synonym(s): *sym*-Dichlorotetrafluoroacetone

CAS Registry Number: 127-21-9

$\text{F}_2\text{CClCOCClF}_2$

Molecular Formula:  $\text{C}_3\text{Cl}_2\text{F}_4\text{O}$

Molecular Weight: 198.931

Accurate Mass: 197.926231

Percentage Composition: C 18.11%; Cl 35.64%; F 38.20%; O 8.04%

Use/Importance: Derivatisation reagent for ms and gc anal. of aminoacid and mandelate esters. Shows fungicidal props.

Physical Description: Liq.

Boiling Point: Bp 44-46°

Solubility: Sol.  $\text{H}_2\text{O}$

Density:  $d_4^{20}$  1.52

Refractive Index:  $n_D^{20}$  1.3300

Hazard & Toxicity: LD<sub>50</sub> (rat, orl) 61 mg/kg. LD<sub>50</sub> (rbt, skn) 91 mg/kg. CNS depressant

Aldrich: D7540-8

Rare Chemicals Library: S43042-0

>>Derivative: Di-Me acetal

Synonym(s): 1,3-Dichloro-1,1,3,3-tetrafluoro-2,2-dimethoxypropane

Molecular Formula:  $\text{C}_5\text{H}_6\text{Cl}_2\text{F}_4\text{O}_2$

Molecular Weight: 245

Accurate Mass: 243.968096

Percentage Composition: C 24.51%; H 2.47%; Cl 28.94%; F 31.02%; O 13.06%

Physical Description: Liq.

Boiling Point: Bp 147-148°

Refractive Index:  $n_D^{20}$  1.3829

>>Derivative: Ethylene acetal

Synonym(s): 2,2-Bis-(*sym*-chlorodifluoromethyl)-1,3-dioxolane

Molecular Formula:  $\text{C}_5\text{H}_4\text{Cl}_2\text{F}_4\text{O}_2$

Molecular Weight: 242.984

Accurate Mass: 241.952446

Percentage Composition: C 24.72%; H 1.66%; Cl 29.18%; F 31.28%; O 13.17%

Physical Description: Liq.

Boiling Point: Bp 171-172°

Refractive Index:  $n_D^{20}$  1.3896

#### References:

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