



>>Entry Name: **3,3-Dibromo-1,1,1-trifluoro-2-propanone**, 9CI

Synonym(s): 3,3-Dibromo-1,1,1-trifluoroacetone

CAS Registry Number: 431-67-4

$\text{F}_3\text{CCOCHBr}_2$

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

Molecular Weight: 269.843

Accurate Mass: 267.874621

Percentage Composition: C 13.35%; H 0.37%; Br 59.22%; F 21.12%; O 5.93%

Physical Description: Liq.

Melting Point: Fp -51°

Boiling Point: Bp $111-113^\circ$

Solubility: Sol. H_2O

Density: d_{20}^{20} 2.19. d 1.4311

Refractive Index: n_D^{20} 1.4311

Hazard & Toxicity: Powerful lachrymator, lung and skin irritant

>>Derivative: Semicarbazone

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 218 dec.°

References:

McBee, E.T. *et al.*, *J.A.C.S.*, 1952, **74**, 3902, (*synth*)

Shapiro, B.L. *et al.*, *J. Magn. Reson.*, 1973, **9**, 305, (*synth, pmr, F-19 nmr*)

Farmer, P.B. *et al.*, *J. Med. Chem.*, 1975, **18**, 1106, (*synth*)