



>>Entry Name: 2-(Trifluoromethyl)-2-propenoic acid, 9CI

Synonym(s): 2-Trifluoromethylacrylic acid

CAS Registry Number: 381-98-6

$\text{H}_2\text{C}=\text{C}(\text{CF}_3)\text{COOH}$

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

Molecular Weight: 140.062

Accurate Mass: 140.008514

Percentage Composition: C 34.30%; H 2.16%; F 40.69%; O 22.85%

Melting Point: Mp 52.5-53° (50-51°)

Boiling Point: Bp 146-148°. Bp₂₈ 90°

Aldrich: 36914-4

>>Derivative: Me ester

CAS Registry Number: 382-90-1

Molecular Formula: $\text{C}_5\text{H}_5\text{F}_3\text{O}_2$

Molecular Weight: 154.088

Accurate Mass: 154.024164

Percentage Composition: C 38.97%; H 3.27%; F 36.99%; O 20.77%

Physical Description: Liq.

Boiling Point: Bp 103.8-105°

Refractive Index: n_D^{20} 1.3370

Other Data: Undergoes anionic homopolym. and radical copolym. Q/e values for copolym., Q 0.74, e +2.5

Hazard & Toxicity: Lachrymator

>>Derivative: Et ester

CAS Registry Number: 87769-68-4

Molecular Formula: $\text{C}_6\text{H}_7\text{F}_3\text{O}_2$

Molecular Weight: 168.115

Accurate Mass: 168.039814

Percentage Composition: C 42.87%; H 4.20%; F 33.90%; O 19.03%

Other Data: Undergoes anionic homopolym.

>>Derivative: Amide

Molecular Formula: $\text{C}_4\text{H}_4\text{F}_3\text{NO}$

Molecular Weight: 139.077

Accurate Mass: 139.024498

Percentage Composition: C 34.54%; H 2.90%; F 40.98%; N 10.07%; O 11.50%

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 104°

>>Derivative: Nitrile

Synonym(s): 2-Trifluoromethylacrylonitrile. 2-Cyano-3,3,3-trifluoropropene

CAS Registry Number: 381-84-0

Molecular Formula: $\text{C}_4\text{H}_2\text{F}_3\text{N}$

Molecular Weight: 121.062

Accurate Mass: 121.013933

Percentage Composition: C 39.69%; H 1.67%; F 47.08%; N 11.57%

Boiling Point: Bp₇₅₉ 75.9-76.2°

Other Data: Undergoes anionic homopolym. and radical copolym.

References:

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Buxton, M.W. *et al.*, *J.C.S.*, 1954, 366
Drakesmith, F.G. *et al.*, *J.O.C.*, 1968, **33**, 280, (synth)
Ito, H. *et al.*, *Macromolecules*, 1982, **15**, 915; 1984, **17**, 2204, (polym, Me ester, nitrile)
Iwatsuki, S. *et al.*, *Macromolecules*, 1984, **17**, 2473, (copolym, reactivity, Me ester, nitrile)
Fuchikami, T. *et al.*, *Synthesis*, 1984, 766, (synth)
Fuchikami, T. *et al.*, *Tet. Lett.*, 1986, **27**, 3173, (deriv, use)
Narita, T. *et al.*, *Polym. J. (Tokyo)*, 1988, **20**, 277, (polym, Et ester)