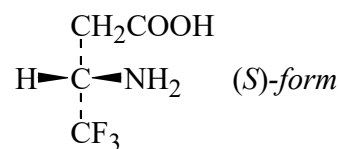




>>Entry Name: 3-Amino-4,4,4-trifluorobutanoic acid

Synonym(s): Trifluoromethyl-β-alanine



CAS Registry Number: 584-20-3

Related CAS Registry Numbers(s): 91291-66-6

Molecular Formula: C₄H₆F₃NO₂

Molecular Weight: 157.092

Accurate Mass: 157.035063

Percentage Composition: C 30.58%; H 3.85%; F 36.28%; N 8.92%; O 20.37%

>>Variant: (S)-form

CAS Registry Number: 128444-38-2

Molecular Formula: C₄H₆F₃NO₂

Molecular Weight: 157.092

Accurate Mass: 157.035063

Percentage Composition: C 30.58%; H 3.85%; F 36.28%; N 8.92%; O 20.37%

Physical Description: Cryst. (EtOH aq) (as hydrochloride)

Melting Point: Mp 204-208° (subl.) (hydrochloride)

Optical Rotation: $[\alpha]_{\text{D}}^{22} +1.4$ (c, 1.1 in MeOH) (50% ee)

pKa Value: pK_{a2} 5.82 (NH₂)

Other Data: CAS no. refers to hydrochloride. Abs. config. not certain owing to translation uncertainty; given as (S)-form in CA

>>Variant: (±)-form

CAS Registry Number: 88968-79-0

Molecular Formula: C₄H₆F₃NO₂

Molecular Weight: 157.092

Accurate Mass: 157.035063

Percentage Composition: C 30.58%; H 3.85%; F 36.28%; N 8.92%; O 20.37%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 189-190 dec.°

References:

Walborsky, H.M. *et al.*, *J.A.C.S.*, 1956, **78**, 4314, (*props*)

Walborsky, H.M. *et al.*, *J.O.C.*, 1956, **21**, 538, (*synth*)

Metcarf, B.W. *et al.*, *Bioorg. Chem.*, 1984, **12**, 91, (*synth*)

Bevilacqua, P.F. *et al.*, *J.O.C.*, 1984, **49**, 1430, (*synth, ir, pmr*)

Wagner, J. *et al.*, *J. Chromatogr.*, 1987, **392**, 211, (*glc*)

Kukhar, V.P. *et al.*, *Dokl. Akad. Nauk SSSR*, 1990, **310**, 886; *Dokl. Chem. (Engl. Transl.)*, 1990, **310**, 26, (*synth, S-form*)