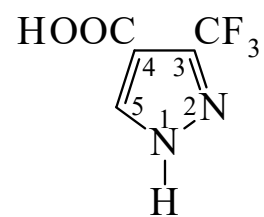




>>Entry Name: 3-Trifluoromethyl-1*H*-pyrazole-4-carboxylic acid



Related CAS Registry Numbers(s): 155377-19-8

Molecular Formula: C₅H₃F₃N₂O₂

Molecular Weight: 180.086

Accurate Mass: 180.014662

Percentage Composition: C 33.35%; H 1.68%; F 31.65%; N 15.56%; O 17.77%

>>Derivative: Me ester

CAS Registry Number: 61859-96-9

Molecular Formula: C₆H₅F₃N₂O₂

Molecular Weight: 194.113

Accurate Mass: 194.030312

Percentage Composition: C 37.13%; H 2.60%; F 29.36%; N 14.43%; O 16.48%

Physical Description: Solid (CHCl₃)

Melting Point: Mp 172-173°

>>Derivative: *N*¹-Me

CAS Registry Number: 113100-53-1

Molecular Formula: C₆H₅F₃N₂O₂

Molecular Weight: 194.113

Accurate Mass: 194.030312

Percentage Composition: C 37.13%; H 2.60%; F 29.36%; N 14.43%; O 16.48%

Physical Description: Cryst. (CHCl₃)

Melting Point: Mp 199-200°

References:

Saunier, Y.H. *et al.*, *Tetrahedron*, 1976, **32**, 1995, (*Me ester, synth, ms, ir, pmr*)

Okada, E. *et al.*, *Heterocycles*, 1992, **34**, 791, (*l-Me, synth, ir, pmr*)

Eur. Pat., 1994, 588 357; *CA*, **121**, 9389h, (*Et ester*)