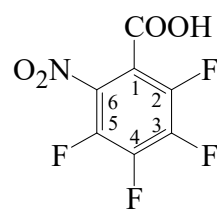




>>Entry Name: 2,3,4,5-Tetrafluoro-6-nitrobenzoic acid, 9CI



CAS Registry Number: 16583-08-7

Related CAS Registry Numbers(s): 103772-10-7

Molecular Formula: C₇HF₄NO₄

Molecular Weight: 239.083

Accurate Mass: 238.984171

Percentage Composition: C 35.17%; H 0.42%; F 31.79%; N 5.86%; O 26.77%

Melting Point: Mp 137-138° (after subl.)

Boiling Point: Subl._{0.2} 130°

>>Derivative: Amide

CAS Registry Number: 16583-07-6

Molecular Formula: C₇H₂F₄N₂O₃

Molecular Weight: 238.098

Accurate Mass: 238.000155

Percentage Composition: C 35.31%; H 0.85%; F 31.92%; N 11.77%; O 20.16%

Physical Description: Cryst. (CHCl₃)

Melting Point: Mp 124-125°

>>Derivative: Nitrile

Synonym(s): 1-Cyano-2,3,4,5-tetrafluoro-6-nitrobenzene

CAS Registry Number: 16583-05-4

Molecular Formula: C₇F₄N₂O₂

Molecular Weight: 220.083

Accurate Mass: 219.98959

Percentage Composition: C 38.20%; F 34.53%; N 12.73%; O 14.54%

Boiling Point: Bp_{0.7} 75-76°

References:

Belf, L.J. *et al.*, *Tetrahedron*, 1967, **23**, 4719-4727, (*synth, amide, nitrile*)

Domagala, J.M. *et al.*, *J. Med. Chem.*, 1991, **34**, 1142-1152, (*synth, ir, pmr*)