



>>Entry Name: 2,6-Difluoro-3-nitrobenzoic acid, 9CI

CAS Registry Number: 83141-10-0

Related CAS Registry Numbers(s): 150368-36-8

Molecular Formula: $C_7H_3F_2NO_4$

Molecular Weight: 203.102

Accurate Mass: 203.003015

Percentage Composition: C 41.40%; H 1.49%; F 18.71%; N 6.90%; O 31.51%

Physical Description: Solid

>>Derivative: Me ester

CAS Registry Number: 84832-01-9

Molecular Formula: $C_8H_5F_2NO_4$

Molecular Weight: 217.129

Accurate Mass: 217.018665

Percentage Composition: C 44.25%; H 2.32%; F 17.50%; N 6.45%; O 29.47%

Physical Description: Cryst.

Melting Point: Mp 56-57°

Boiling Point: Bp₉ 149-151°

References:

Tani, J. *et al.*, *Chem. Pharm. Bull.*, 1982, **30**, 3530-3543, (*synth, pmr*)

Soundararajan, N. *et al.*, *J.O.C.*, 1990, **55**, 2034-2044, (*synth, ir, pmr, F-19 nmr, ms*)

Kim, K.S. *et al.*, *J. Med. Chem.*, 1993, **36**, 2335-2342, (*Et ester, synth, pmr*)

Yoshida, Y. *et al.*, *Bioorg. Med. Chem.*, 1999, **7**, 2647-2666, (*synth, pmr*)