



>>Entry Name: 4-Amino-2-fluorobenzoic acid

CAS Registry Number: 446-31-1

Molecular Formula: $C_7H_6FNO_2$

Molecular Weight: 155.128

Accurate Mass: 155.038257

Percentage Composition: C 54.20%; H 3.90%; F 12.25%; N 9.03%; O 20.63%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 216-216.5°

>>Derivative: Me ester

Molecular Formula: $C_8H_8FNO_2$

Molecular Weight: 169.155

Accurate Mass: 169.053907

Percentage Composition: C 56.80%; H 4.77%; F 11.23%; N 8.28%; O 18.92%

Physical Description: Cryst. solid

Melting Point: Mp 108-110°

>>Derivative: *tert*-Butyl ester

Molecular Formula: $C_{11}H_{14}FNO_2$

Molecular Weight: 211.235

Accurate Mass: 211.100857

Percentage Composition: C 62.55%; H 6.68%; F 8.99%; N 6.63%; O 15.15%

Physical Description: Pale yellow solid

Melting Point: Mp 103°

>>Derivative: *N*-Ac

Molecular Formula: $C_9H_8FNO_3$

Molecular Weight: 197.165

Accurate Mass: 197.048822

Percentage Composition: C 54.83%; H 4.09%; F 9.64%; N 7.10%; O 24.34%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 256-257°

>>Derivative: *N*-Me

Synonym(s): 2-Fluoro-4-methylaminobenzoic acid

CAS Registry Number: 173951-99-0

Molecular Formula: $C_8H_8FNO_2$

Molecular Weight: 169.155

Accurate Mass: 169.053907

Percentage Composition: C 56.80%; H 4.77%; F 11.23%; N 8.28%; O 18.92%

Physical Description: Solid

Melting Point: Mp 184-186°

>>Derivative: *N*-Me, *tert*-butyl ester

CAS Registry Number: 153538-28-4

Molecular Formula: $C_{12}H_{16}FNO_2$

Molecular Weight: 225.262

Accurate Mass: 225.116507

Percentage Composition: C 63.98%; H 7.16%; F 8.43%; N 6.22%; O 14.21%

Physical Description: Solid

Melting Point: Mp 76-78°

>>Derivative: *N*-Trifluoroacetyl, *tert*-Butyl ester

Molecular Formula: $C_{13}H_{13}F_4NO_3$

Molecular Weight: 307.244

Accurate Mass: 307.083156

Percentage Composition: C 50.82%; H 4.26%; F 24.73%; N 4.56%; O 15.62%

Physical Description: Oil

References: