



>>Entry Name: 4-Amino-3,5-dinitrobenzoic acid, 9CI

Synonym(s): Chrysanic acid, 8CI

CAS Registry Number: 7221-27-4

Molecular Formula: $C_7H_5N_3O_6$

Molecular Weight: 227.133

Accurate Mass: 227.017837

Percentage Composition: C 37.02%; H 2.22%; N 18.50%; O 42.26%

Physical Description: Yellow leaflets (EtOH)

Melting Point: Mp 259°

>>Derivative: Me ester

CAS Registry Number: 54226-20-9

Molecular Formula: $C_8H_7N_3O_6$

Molecular Weight: 241.16

Accurate Mass: 241.033487

Percentage Composition: C 39.84%; H 2.93%; N 17.42%; O 39.81%

Melting Point: Mp 144°

>>Derivative: Et ester

CAS Registry Number: 54226-19-6

Molecular Formula: $C_9H_9N_3O_6$

Molecular Weight: 255.187

Accurate Mass: 255.049137

Percentage Composition: C 42.36%; H 3.55%; N 16.47%; O 37.62%

Melting Point: Mp 114°

>>Derivative: Amide

CAS Registry Number: 54321-79-8

Molecular Formula: $C_7H_6N_4O_5$

Molecular Weight: 226.148

Accurate Mass: 226.033821

Percentage Composition: C 37.18%; H 2.67%; N 24.77%; O 35.37%

Physical Description: Yellow needles (MeCN)

Melting Point: Mp 259°

>>Derivative: *N,N*-Di-Me

CAS Registry Number: 82366-55-0

Molecular Formula: $C_9H_9N_3O_6$

Molecular Weight: 255.187

Accurate Mass: 255.049137

Percentage Composition: C 42.36%; H 3.55%; N 16.47%; O 37.62%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 248°

References:

Lindermann, H. *et al.*, *Ber.*, 1925, **58**, 1221, (*amide, synth*)

Jensen, K.A. *et al.*, *Acta Chem. Scand.*, 1950, **4**, 392, (*N,N-di-Me*)

Cosulich, D.B. *et al.*, *J.A.C.S.*, 1953, **75**, 4675, (*synth*)