



>>Entry Name: 4-Nitro-1,8-naphthalenedicarboxylic acid, 9CI

Synonym(s): 4-Nitronaphthalic acid, 8CI

CAS Registry Number: 5425-83-2

Molecular Formula: C<sub>12</sub>H<sub>7</sub>NO<sub>6</sub>

Molecular Weight: 261.19

Accurate Mass: 261.027339

Percentage Composition: C 55.18%; H 2.70%; N 5.36%; O 36.75%

Physical Description: Yellow cryst.

Other Data: Readily forms the anhydride on heating. Dec. at 140-50°.

>>Derivative: Di-Me ester

CAS Registry Number: 30084-57-2

Molecular Formula: C<sub>14</sub>H<sub>11</sub>NO<sub>6</sub>

Molecular Weight: 289.244

Accurate Mass: 289.058639

Percentage Composition: C 58.14%; H 3.83%; N 4.84%; O 33.19%

Physical Description: Cryst.

Melting Point: Mp 125-126°

>>Derivative: Di-Et ester

CAS Registry Number: 30084-59-4

Molecular Formula: C<sub>16</sub>H<sub>15</sub>NO<sub>6</sub>

Molecular Weight: 317.298

Accurate Mass: 317.089939

Percentage Composition: C 60.57%; H 4.76%; N 4.41%; O 30.25%

Physical Description: Yellow-green cryst.

Melting Point: Mp 86°

>>Derivative: Anhydride

CAS Registry Number: 6642-29-1

Molecular Formula: C<sub>12</sub>H<sub>5</sub>NO<sub>5</sub>

Molecular Weight: 243.175

Accurate Mass: 243.016774

Percentage Composition: C 59.27%; H 2.07%; N 5.76%; O 32.90%

Physical Description: Cryst. (AcOH or HNO<sub>3</sub>)

Melting Point: Mp 228-229°

Rare Chemicals Library: S26596-9

>>Derivative: Imide

Molecular Formula: C<sub>12</sub>H<sub>6</sub>N<sub>2</sub>O<sub>4</sub>

Molecular Weight: 242.19

Accurate Mass: 242.032758

Percentage Composition: C 59.51%; H 2.50%; N 11.57%; O 26.42%

Physical Description: Cryst.

Melting Point: Mp 284°

#### References:

Graebe, C. *et al.*, *Annalen*, 1903, **327**, 77

Dziewonski, K., *Ber.*, 1903, **36**, 3768

Jones, L.A. *et al.*, *Can. J. Chem.*, 1970, **48**, 3132

Grayshan, P.H. *et al.*, *J.C.S.(C)*, 1971, 3599

Petrenko, G.P. *et al.*, *Zh. Obshch. Khim.*, 1974, **10**, 1950