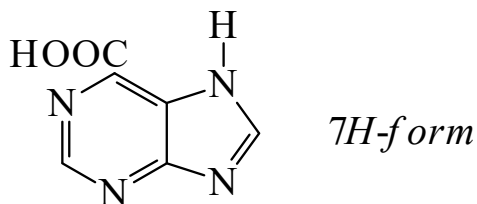




>>Entry Name: 6-Purinecarboxylic acid

Synonym(s): Purinoic acid



CAS Registry Number: 2365-43-7

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

Molecular Weight: 164.123

Accurate Mass: 164.033426

Percentage Composition: C 43.91%; H 2.46%; N 34.14%; O 19.50%

Physical Description: Cryst. (H<sub>2</sub>O)

Melting Point: Mp 200-202°

Sigma: C6006

>>Derivative: Et ester

CAS Registry Number: 40769-66-2

Molecular Formula: C<sub>8</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>

Molecular Weight: 192.177

Accurate Mass: 192.064726

Percentage Composition: C 50.00%; H 4.20%; N 29.15%; O 16.65%

Melting Point: Mp 160-161°

>>Derivative: Amide

CAS Registry Number: 37527-29-0

Molecular Formula: C<sub>6</sub>H<sub>5</sub>N<sub>5</sub>O

Molecular Weight: 163.138

Accurate Mass: 163.04941

Percentage Composition: C 44.17%; H 3.09%; N 42.93%; O 9.81%

Physical Description: Cryst. (H<sub>2</sub>O)

Melting Point: Mp 315-320°

>>Derivative: Nitrile

CAS Registry Number: 2036-13-7

Molecular Formula: C<sub>6</sub>H<sub>3</sub>N<sub>5</sub>

Molecular Weight: 145.123

Accurate Mass: 145.038845

Percentage Composition: C 49.66%; H 2.08%; N 48.26%

Physical Description: Cryst. (C<sub>6</sub>H<sub>6</sub>)

Melting Point: Mp 177-178°. Mp 186-189°

Aldrich: 85250-3

Rare Chemicals Library: S44915-6

Sigma: C5392

#### References:

Mackay, L.B. *et al.*, *J.A.C.S.*, 1956, **78**, 3511, (*synth, amide*)

Giner-Sorolla, A., *Chem. Ber.*, 1968, **101**, 611, (*synth*)

Hampton, A., *J. Het. Chem.*, 1974, **11**, 255, (*synth*)

Prendergast, W. *et al.*, *J. Het. Chem.*, 1989, 1863, (*synth, pmr, derivs*)