



>>Entry Name: Phenylguanidine, 9CI

CAS Registry Number: 2002-16-6
HN=C(NH2)NHPH<<>>(H2N)2C=NPh

Molecular Formula: C₇H₉N₃
Molecular Weight: 135.168
Accurate Mass: 135.079647
Percentage Composition: C 62.20%; H 6.71%; N 31.09%

Physical Description: Cryst. (C₆H₆)
Melting Point: Mp 66-67°
Solubility: Spar. sol. H₂O
pKa Value: pK_a 10.77 (25°)

Rare Chemicals Library: S82006-7

>>Derivative: Hydrochloride

CAS Registry Number: 6522-91-4
Physical Description: Hygroscopic cryst.
Melting Point: Mp 76°

>>Derivative: Hydrobromide

Melting Point: Mp 71°

>>Derivative: Nitrate

CAS Registry Number: 18860-78-1
Physical Description: Needles or prisms
Melting Point: Mp 128°

>>Derivative: *N*-Benzoyl

Molecular Formula: C₁₄H₁₃N₃O
Molecular Weight: 239.276
Accurate Mass: 239.105862
Percentage Composition: C 70.28%; H 5.48%; N 17.56%; O 6.69%
Physical Description: Pale-yellow prisms (C₆H₆/petrol)
Melting Point: Mp 91-92°

>>Derivative: *N*-Benzoyl, picrate

Physical Description: Yellow prisms (EtOH)
Melting Point: Mp 186°

>>Derivative: *N,N'*-Bis(methoxycarbonyl)

CAS Registry Number: 136437-04-2
Molecular Formula: C₁₁H₁₃N₃O₄
Molecular Weight: 251.241
Accurate Mass: 251.090607
Percentage Composition: C 52.59%; H 5.22%; N 16.72%; O 25.47%
Physical Description: Cryst. (C₆H₆/petrol)
Melting Point: Mp 180-182.5°

References:

- Smith, G.B.L., *J.A.C.S.*, 1929, **51**, 477, (*synth*)
Scott, F.L. *et al.*, *J.O.C.*, 1956, **21**, 1519, (*synth*)
Hirt, R.C. *et al.*, *Spectrochim. Acta*, 1959, **15**, 962, (*uv*)
Bredereck, H. *et al.*, *Chem. Ber.*, 1965, **98**, 3178, (*synth*)
Botto, R.E. *et al.*, *Proc. Natl. Acad. Sci. U.S.A.*, 1980, **77**, 23, (*cmr*)
Palát, K. *et al.*, *Coll. Czech. Chem. Comm.*, 1992, **57**, 1127, (*deriv*)