



>>Entry Name: *N,N'*-Diphenylguanidine, 9CI

Synonym(s): 1,3-Diphenylguanidine, 8CI. Accelerator D. Melaniline. Phenaldine. DPG

CAS Registry Number: 102-06-7

Type of Compound Code(s): PS7700 PS8300 PA5010

HN=C(NHPh)₂

Molecular Formula: C₁₃H₁₃N₃

Molecular Weight: 211.266

Accurate Mass: 211.110947

Percentage Composition: C 73.91%; H 6.20%; N 19.89%

Use/Importance: Vulcanisation accelerator, complexing agent in detection of metals, organic base. Used as protonated form (diphenylguanidinium ion); forms extractable ion-pairs with anionic complexes of metals, e.g. Co, Ga, In, Mo, Rh, Sn, Ti, V, W, for extraction separation and photometric detn.

Physical Description: Needles (EtOH)

Melting Point: Mp 150°

Solubility: Sol. Et₂O, CHCl₃, dil. acids; spar. sol. H₂O

pKa Value: pK_a 10.12 (25°, H₂O)

Other Data: Strongly alkaline soln.

Hazard & Toxicity: Irritant. Highly toxic orally. LD₅₀ (mus, orl) 290 mg/kg. LD₅₀ (rat, orl) 507 mg/kg. Exp. reprod. and teratogenic effects

Aldrich: D20775-6

Fluka: 43030

>>Derivative: Hydrochloride

CAS Registry Number: 24245-27-0

Melting Point: Mp 137.5°

>>Derivative: Hydrobromide

Physical Description: Solid

Melting Point: Mp 158-160°

>>Derivative: Perchlorate

CAS Registry Number: 18720-54-2

Melting Point: Mp 161-163°

>>Derivative: Nitrate

CAS Registry Number: 104083-00-3

Physical Description: Cryst.

Melting Point: Mp 195-196 dec.°

>>Derivative: Picrate

Physical Description: Cryst.

Melting Point: Mp 171°

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

Synonym(s): *N,N'*-Dimethyl-*N,N'*-diphenylguanidine

Molecular Formula: C₁₅H₁₇N₃

Molecular Weight: 239.319

Accurate Mass: 239.142247

Percentage Composition: C 75.28%; H 7.16%; N 17.56%

Physical Description: Oil, cryst. + 2H₂O (hexane <-20°)

References: