



>>Entry Name: **2,5-Di-*tert*-butylaniline**, 8Cl
Synonym(s): 2,5-Bis(1,1-dimethylethyl)benzenamine, 9Cl

CAS Registry Number: 21860-03-7
Related CAS Registry Numbers(s): 118056-75-0

Molecular Formula: C₁₄H₂₃N
Molecular Weight: 205.342
Accurate Mass: 205.183049
Percentage Composition: C 81.89%; H 11.29%; N 6.82%
Physical Description: Fine long needles (EtOH)
Melting Point: Mp 104-104.8°
pKa Value: pK_a 3.58 (25°,50% EtOH)

Aldrich: 27573-5
Fluka: 34560

>>Derivative: Nitrate

CAS Registry Number: 22545-36-4
Physical Description: Cryst. (C₆H₆/petrol or AcOH)
Melting Point: Mp 188-189°

>>Derivative: *N*-Ac

Molecular Formula: C₁₆H₂₅NO
Molecular Weight: 247.38
Accurate Mass: 247.193614
Percentage Composition: C 77.68%; H 10.19%; N 5.66%; O 6.47%
Physical Description: Solid
Melting Point: Mp 155.6-156.4°

>>Derivative: *N*-Benzoyl

Molecular Formula: C₂₁H₂₇NO
Molecular Weight: 309.45
Accurate Mass: 309.209264
Percentage Composition: C 81.51%; H 8.79%; N 4.53%; O 5.17%
Physical Description: Solid
Melting Point: Mp 202.3-203°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 497A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1135C, (*ir*)
Bartlett, P.D. *et al.*, *J.A.C.S.*, 1954, **76**, 2349, (*synth*)
Burgers, J. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1958, **77**, 491, (*synth, uv*)
Krueger, P.J. *et al.*, *Can. J. Chem.*, 1962, **40**, 2300, (*ir*)
Bantel, K.H. *et al.*, *Chem. Ber.*, 1969, **102**, 696, (*synth*)