



>>Entry Name: Azobenzene-3-carboxylic acid

Synonym(s): 3-Phenylazobenzoic acid, 9Cl. *m*-Phenylazobenzoic acid, 8Cl. Benzeneazo-*m*-benzoic acid

CAS Registry Number: 14474-22-7

Molecular Formula: C₁₃H₁₀N₂O₂

Molecular Weight: 226.234

Accurate Mass: 226.074228

Percentage Composition: C 69.02%; H 4.46%; N 12.38%; O 14.14%

>>Variant: (*E*)-(?) -form

CAS Registry Number: 37790-19-5

Molecular Formula: C₁₃H₁₀N₂O₂

Molecular Weight: 226.234

Accurate Mass: 226.074228

Percentage Composition: C 69.02%; H 4.46%; N 12.38%; O 14.14%

Physical Description: Orange cryst. (EtOH)

Melting Point: Mp 170-171°

>>Derivative: Me ester

CAS Registry Number: 24599-38-0

Molecular Formula: C₁₄H₁₂N₂O₂

Molecular Weight: 240.261

Accurate Mass: 240.089878

Percentage Composition: C 69.99%; H 5.03%; N 11.66%; O 13.32%

Physical Description: Yellow leaflets (MeOH)

Melting Point: Mp 58°

>>Derivative: Amide

CAS Registry Number: 29530-52-7

Molecular Formula: C₁₃H₁₁N₃O

Molecular Weight: 225.249

Accurate Mass: 225.090212

Percentage Composition: C 69.32%; H 4.92%; N 18.65%; O 7.10%

Physical Description: Orange leaflets (EtOH)

Melting Point: Mp 205° (199-198°)

>>Derivative: Nitrile

Synonym(s): 3-Cyanoazobenzene

CAS Registry Number: 55669-57-3

Molecular Formula: C₁₃H₉N₃

Molecular Weight: 207.234

Accurate Mass: 207.079647

Percentage Composition: C 75.35%; H 4.38%; N 20.28%

Melting Point: Mp 90.5-91°

References:

Badger, G.M. *et al.*, *Aust. J. Chem.*, 1964, **17**, 1036-1049, (*synth*)

Bowie, J.H. *et al.*, *J.C.S.(B)*, 1967, 621-628, (*ms*)

Roling, P.V. *et al.*, *J.O.C.*, 1975, **40**, 2421-2425, (*nitrile, synth, ir, pmr*)

Rudesinsky, M. *et al.*, *Magn. Reson. Chem.*, 1989, **27**, 585-591, (*Me ester, cmr*)

Vogtle, F. *et al.*, *Chem. Eur. J.*, 1998, **4**, 699-706, (*amide, synth, ms*)