



>>Entry Name: 2-Amino-5-nitrobenzophenone, 8Cl

Synonym(s): (2-Amino-5-nitrophenyl)phenylmethanone, 9Cl. 2-Benzoyl-4-nitroaniline

CAS Registry Number: 1775-95-7

Molecular Formula: C<sub>13</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>

Molecular Weight: 242.234

Accurate Mass: 242.069143

Percentage Composition: C 64.46%; H 4.16%; N 11.56%; O 19.81%

Use/Importance: Precursor of benzodiazepine derivatives, and metab. of Nitrazepam [FTT90-V](#)

Physical Description: Orange prisms with blue reflex (EtOAc)

Melting Point: Mp 161.5°

Aldrich: 21173-7

>>Derivative: (E)-Oxime

Molecular Formula: C<sub>13</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>

Molecular Weight: 257.248

Accurate Mass: 257.080042

Percentage Composition: C 60.70%; H 4.31%; N 16.33%; O 18.66%

Use/Importance: Benzodiazepine precursor

Melting Point: Mp 200-206°

>>Derivative: N-Me

CAS Registry Number: 4958-56-9

Molecular Formula: C<sub>14</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>

Molecular Weight: 256.26

Accurate Mass: 256.084793

Percentage Composition: C 65.62%; H 4.72%; N 10.93%; O 18.73%

Melting Point: Mp 161-163°

Rare Chemicals Library: S1215-8

#### References:

*Aldrich Library of NMR Spectra*, 2nd edn., 1983, **2**, 77D; 78A

*Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **2**, 73B; 73C, (*ir*)

Ullmann, F., *Ber.*, 1898, **31**, 1695, (*synth*)

Nelson, A.L., *Chem. Ind. (London)*, 1965, 653, (*synth*)

*Netherlands Pat.*, 1965, 6 504 628; *CA*, **64**, 8205, (*oximes*)

Ayyangar, N.R. *et al.*, *Org. Prep. Proced. Int.*, 1987, **19**, 167, (*synth, bibl*)

Cox, P.J. *et al.*, *Acta Cryst. C*, 1998, **54**, 856-859, (*cryst struct*)