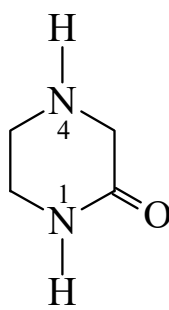




>>Entry Name: Piperazinone, 9CI

Synonym(s): 2-Ketopiperazine



CAS Registry Number: 5625-67-2

Molecular Formula: C₄H₈N₂O

Molecular Weight: 100.12

Accurate Mass: 100.063663

Percentage Composition: C 47.99%; H 8.05%; N 27.98%; O 15.98%

Physical Description: Cryst. (Me₂CO/petrol)

Melting Point: Mp 136°

>>Derivative: N¹-Ph

Synonym(s): 1-Phenyl-2-piperazinone

CAS Registry Number: 94783-18-3

Molecular Formula: C₁₀H₁₂N₂O

Molecular Weight: 176.218

Accurate Mass: 176.094963

Percentage Composition: C 68.16%; H 6.86%; N 15.90%; O 9.08%

Physical Description: Cryst. (Et₂O/hexane)

Melting Point: Mp 93-94°

>>Derivative: N⁴-Benzyl

CAS Registry Number: 13754-41-1

Molecular Formula: C₁₁H₁₄N₂O

Molecular Weight: 190.244

Accurate Mass: 190.110613

Percentage Composition: C 69.45%; H 7.42%; N 14.72%; O 8.41%

Physical Description: Prisms (C₆H₆)

Melting Point: Mp 155-157° (149-150°)

References:

Aspinall, S.R., *J.A.C.S.*, 1940, **62**, 1202-1204, (*synth*)

Uchida, H. *et al.*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 3612-3613, (*N⁴-benzyl, synth*)

Nate, H. *et al.*, *Chem. Pharm. Bull.*, 1987, **35**, 2825-2839, (*N¹-Ph, synth, ir, pmr*)

Choi, S.-W. *et al.*, *J. Med. Chem.*, 1999, **42**, 3647-3656, (*synth, pmr, cmr*)