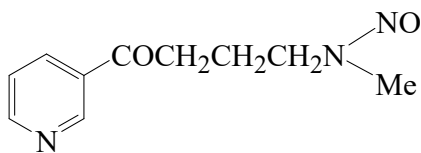




>>Entry Name: 4-(Methylnitrosoamino)-1-(3-pyridinyl)-1-butanone, 9CI

Synonym(s): NNK



CAS Registry Number: 64091-91-4

Molecular Formula: C₁₀H₁₃N₃O₂

Molecular Weight: 207.232

Accurate Mass: 207.100777

Percentage Composition: C 57.96%; H 6.32%; N 20.28%; O 15.44%

Biological Source: Found in tobacco products

Use/Importance: Implicated in oral cancer amongst smokeless tobacco users. Human metab. of nicotine from cigarette smoke

Physical Description: Cryst. (CH₂Cl₂/Et₂O)

Melting Point: Mp 71-73°

Hazard & Toxicity: Carcinogen

>>Derivative: Alcohol

Synonym(s): 4-(Methylnitrosoamino)-1-(3-pyridinyl)-1-butanol. α-[3-(Methylnitrosoamino)propyl]-3-pyridinemethanol, 9CI

CAS Registry Number: 76014-81-8

Extra CAS Registry Numbers(s): 148507-86-2

Molecular Formula: C₁₀H₁₅N₃O₂

Molecular Weight: 209.247

Accurate Mass: 209.116427

Percentage Composition: C 57.40%; H 7.23%; N 20.08%; O 15.29%

Biological Source: Metab. of the ketone

Hazard & Toxicity: Carcinogenic in rats

References:

Hecht, S.S. *et al.*, *J.O.C.*, 1978, **43**, 72-76, (*synth*)

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Pathak, T. *et al.*, *Tetrahedron*, 1990, **46**, 1733-1744, (*synth, pmr, cmr, ms*)

Prokopczyk, B. *et al.*, *Carcinogenesis (London)*, 1992, **13**, 863-866, (*glc*)

Hecht, S.S. *et al.*, *N. Engl. J. Med.*, 1993, **329**, 1543-1546, (*metab, anal*)

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Sax, N.I. *et al.*, *Dangerous Properties of Industrial Materials*, 7th edn., Van Nostrand Reinhold, 1989, MMS250, (*tox*)