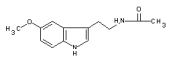

Formula: C13H16N2O2

MW: 232.28

CAS: 73-31-4

MDL: MFCD00005655

TNP: TNP00300

Acetamide, N-[2-(5-methoxy-1H-indol-3-yl)ethyl]-; Acetamide, N-[2-(5-methoxyindol-3-yl)ethyl]-; Acetamide,N-[2-(5-methoxy-1H-indol-3-yl)ethyl]; Melatonin(N-Acetyl-5-methoxytryptamine); n-(2-(5-methoxy-1h-indol-3-yl)ethyl)-acetamid; n-(2-(5-methoxyindol-3-yl)et

LogP: 1.59

LogS: -3.4

Acceptors: 2

Donors: 2

Rotation Bonds: 4

Chiral Centers: 0

N+O: 4

LIPINSKY: 4

IUPAC: N-[2-(5-methoxyindol-3-yl)ethyl]acetamide

Smiles: [nH]1c2c(c(c1)CCNC(=O)C)cc(cc2)OC

Specification: Heterocyclic Series; Heterocycles series; Indoles; Tryptamines; Nutritional Supplements; Intermediates & Fine Chemicals; Pharmaceuticals; Melatonin receptor

Melatonine Chemical Properties:

mp 116.5-118 C(lit.) storage temp. -15C Merck 5816 CAS DataBase Reference73-31-4(CAS DataBase Reference) NIST Chemistry ReferenceMelatonin(73-31-4) Safety Information Hazard Codes T Risk Statements 60 Safety Statements 24/25-99-53-45 WGK Germany 2 RTECS AC5955000 F 8-10-23 HS Code 29379000 Hazardous Substances Data73-31-4(Hazardous Substances Data) Melatonine English Melatonine Usage And Synthesis Chemical Properties:

Off-White Powder UsageHormone postulated to mediate photoperiodicity in mammals. Inhibits cerebellar nitric oxide synthetase Biological ActivityEndogenous hormone that acts as an agonist at melatonin receptors MT 1 and MT 2 . Exhibits a prominent role in the control of circadian rhythm, displays immunomodulatory activity and acts as a powerful antioxidant in vivo . Melatonine

Merck 13 Reference: Monograph Number: 0005838

Title: Melatonin

CAS Registry Number: 73-31-4

CAS Name: N-[2-(5-Methoxy-1H-indol-3-yl)ethyl]acetamide

Additional Names: N-acetyl-5-methoxytryptamine

Trademarks: Regulin (Young)

Molecular Formula: C13H16N2O2

Molecular Weight: 232.28.

Percent Composition: C 67.22%, H 6.94%, N 12.06%, O 13.78%

Literature References: A hormone of the pineal gland, also produced by extra-pineal tissues, that lightens skin color in amphibians by reversing the darkening effect of MSH, q.v. Melatonin has been postulated as the mediator of photic-induced antigonadotrophic activity in photoperiodic mammals and has also been shown to be involved in thermoregulation in some ectotherms and in affecting locomotor activity rhythms in sparrows. Isoln from the pineal glands of beef cattle: Lerner et al., J. Am. Chem. Soc. 80, 2587 (1958); Wurtman et al., Science 141, 277 (1963). Structure: Lerner et al., J. Am. Chem. Soc. 81, 6084 (1959). Crystal and molecular structure: A. Wakahara, Chem. Lett. 1972, 1139. Synthesis from 5-methoxyindole as starting material by two different routes: Szmuszkovicz et al., J. Org. Chem. 25, 857 (1960). Biochemical role of melatonin: Chem. Eng. News 45, 40 (May 1, 1967). Pharmacological studies: Barchas et al., Nature 214, 919 (1967). Identification of antigonadal action sites in mouse brain: J. D. Glass, G. R. Lynch, Science 214, 821 (1981). Binding studies in human hypothalamus: S. M. Reppert et al., Science 242, 78 (1988). Efficacy in control of estrus in red deer: G. W. Asher, Anim. Reprod. Sci. 22, 145 (1990). Reviews: M. K. Vaughn, Int. J. Rev.

Physiol. 24, 41-95 (1981); D. C.Klein et al., Life Sci. 28, 1975-1986 (1981). Book: Advan. Biosci. vol. 29, N. Birau, W. Schlott, Eds. (Pergamon Press, New York, 1981) 420 pp. Review of etiological role in clinical disease: A. Miles, D. Philbrick, Crit. Rev. Clin. Lab. Sci. 25, 231-253 (1987); in psychiatric disorders: eidem, Biol. Psychiatry 23, 405-425 (1988).

Properties: Pale yellow leaflets from benzene, mp 116-118. uv max: 223, 278 nm (e 27550, 6300).

Melting point: mp 116-118

Absorption maximum: uv max: 223, 278 nm (e 27550, 6300)

Therap-Cat-Vet: Control of estrus.