



Formula: C₁₈H₂₇NO₃

MW: 305.42

CAS: 404-86-4

TNP NUMBER: TNP00277

MDL NUMBER: MFCD00017259

IUPAC: (6E)-N-[(4-hydroxy-3-methoxyphenyl)methyl]-8-methylnon-6-enamide

Smiles: C(NC(CCCCC=CC(C)C)=O)c1cc(OC)c(cc1)O

Pungent principle in fruit of various species of Capsicum, Solanaceae

THERAPEUTIC CATEGORY: Topical analgesic

ACCEPTORS: 3

DONORS: 2

ROTATION BONDS: 10

N+O: 4

Chiral Centers: 0

LogP: 4.19

LogS: -4.6

LIPINSKI: 4

Monograph Number: 0001774

Title: Capsaicin

CAS Registry Number: 404-86-4

CAS Name: (6E)-N-[(4-Hydroxy-3-methoxyphenyl)methyl]-8-methyl-6-nonenamide

Additional Names: trans-8-methyl-N-vanillyl-6-nonenamide;
N-(4-hydroxy-3-methoxybenzyl)-8-methylnon-trans-6-enamide

Trademarks: Axsain (Bioglan); Mioton (Pharmakhim); Zacin (Bioglan); Zostrix (GenDerm)

Molecular Formula: C₁₈H₂₇NO₃

Molecular Weight: 305.41.

Percent Composition: C 70.79%, H 8.91%, N 4.59%, O 15.72%

Literature References: Pungent principle in fruit of various species of *Capsicum*, Solanaceae. Isolated from paprika and cayenne: Thresh, *Pharm. J. Trans.* 7, 21 (1876); Micko, *Z. Nahr. Genussm.* 1, 818 (1898). See Beilstein 13, suppl. I, 322. Early structure study: Nelson, *J. Am. Chem. Soc.* 42, 597 (1920). Synthesis: Spath, *Darling, Ber.* 63, 737 (1930); L. Crombie et al., *J. Chem. Soc.* 1955, 1025; O. P. Vig et al., *Indian J. Chem.* 17B, 558 (1979). Constitution and biosynthesis: D. J. Bennet, E. W. Kirby, *J. Chem. Soc. C* 1968, 442. Pharmacology: J. Molnar et al., *Acta Physiol. Acad. Sci. Hung.* 35, 369 (1969). Capsaicin is a powerful irritant; initial administration causes intense pain. Prolonged treatment causes insensitivity to painful stimuli and induces selective degeneration of certain primary sensory neurons: G. Jancso et al., *Nature* 270, 741 (1977); R. Gamse, *Arch. Pharmacol.* 320, 205 (1982); P. Holzer et al., *Neurosci. Lett.* 31, 253 (1982). Neuronal depletion of substance P, q.v.: T. M. Jessell et al., *Brain Res.* 152, 183 (1978); T. L. Yaksh et al., *Science* 206, 481 (1979). Capsaicin pretreatment also induces long-lasting desensitization of airway mucosa to various mechanical and chemical irritants: J. M. Lundberg, A. Saria, *Nature* 302, 251 (1983). Preliminary clinical evaluation in chronic postherpetic neuralgia: J. E. Bernstein et al., *J. Am. Acad. Dermatol.* 17, 93 (1987). Reviews: Molnar, *Arzneim.-Forsch.* 15, 718 (1965); Walker, *Gavern, Manuf. Chem. Aerosol News* 39 (6), 35 (1968); R. M. Virus, G. F. Gebhart, *Life Sci.* 25, 1273 (1979); Y. Monsereenusorn et al., *Crit. Rev. Toxicol.* 10, 321-339 (1982).

Properties: Monoclinic, rectangular plates, scales from petr ether, mp 65. bp0.01 210-220 (air-bath temp). uv max: 227, 281 nm (e 7000, 2500). Burning taste, one part in 100,000 can be detected by tasting. Practically insol in cold water. Freely sol in alc, ether, benzene, chloroform; slightly sol in CS₂.

Melting point: mp 65

Boiling point: bp0.01 210-220 (air-bath temp)

Absorption maximum: uv max: 227, 281 nm (e 7000, 2500)

Use: As a tool in neurobiological research.

Therap-Cat: Topical analgesic.

Therap-Cat-Vet: Topical analgesic.

Synonyms: (E)-8-METHYL-NON-6-ENOIC ACID
4-HYDROXY-3-METHOXY-BENZYLAMIDE;(E)-CAPSAICIN;(E)-N-[(4-HYDROXY-3-METHOXY
PHENYL]METHYL)8-METHYL-6-NONEAMIDE;(E)-N-[(4-HYDROXY-3-METHOXYPHENYL)ME
THYL]-8-METHYL-6-NONENAMIDE;CAPSAICIN;CAPSAICINE;CAPSAICIN, NATURAL;FEMA
3404

CAS:404-86-4

MF:C18H27NO3

MW:305.41

EINECS:206-969-8

Product Categories:INORGANIC & ORGANIC CHEMICALS;Anilines, Aromatic Amines and
Nitro Compounds;Miscellaneous Natural Products;Natural Plant Extract;Intermediates & Fine
Chemicals;Pharmaceuticals;Vanilloid/TRPV channel Capsaicin

Chemical Properties: mp 62-65 C(lit.) bp 210-220 C FEMA 3404 Fp 113 C storage temp. 2-8C
solubility H2O: insoluble Water Solubility insoluble Merck 1768 Stability:Stable. Incompatible
with strong oxidizing agents.

CAS DataBase Reference: 404-86-4(

CAS DataBase Reference:) EPA Substance Registry System6-Nonenamide,
N-[(4-hydroxy-3-methoxyphenyl) methyl]-8-methyl-, (6E)-(404-86-4) T,T+ Risk Statements
25-37/38-41-42/43-36/37/38 Safety Statements 22-26-28-36/39-45-36/37/39 RIDADR UN 2811
6.1/PG 2 WGK Germany 3 RTECS RA8530000 F 10-21 HazardClass 6.1(a) PackingGroup II
Hazardous Substances Data404-86-4(Hazardous Substances Data)
(E)-N-[(4-Hydroxy-3-methoxyphenyl)methyl]-8-methyl-6-nonenamide Capsaicin

Usage And Synthesis:

Chemical Properties: Off-White Crystalline Solid UsageA representative lot is a 5:1 E:Z mixture.

It is used as a tool in neurobiological research. Prototypic vanilloid receptor agonist. Topical analgesic. Biological Activity Prototypic vanilloid receptor agonist (pEC 50 values are 7.97 and 7.10 at rat and human VR1 receptors respectively). Excites a subset of primary afferent sensory neurons, with subsequent antinociceptive and anti-inflammatory effects. Reversibly inhibits aggregation of platelets. Also available as part of the Vanilloid TRPV1 Receptor Tocriset .
Capsaicin

