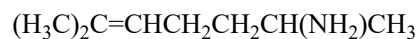




>>Entry Name: 6-Methyl-5-hepten-2-amine, 9Cl

Synonym(s): 1,5-Dimethyl-4-hexenylamine, 8Cl. 6-Amino-2-methyl-2-heptene. Isooctenylamine



Molecular Formula: C₈H₁₇N

Molecular Weight: 127.229

Accurate Mass: 127.136099

Percentage Composition: C 75.52%; H 13.47%; N 11.01%

>>Variant: (±)-form

Molecular Formula: C₈H₁₇N

Molecular Weight: 127.229

Accurate Mass: 127.136099

Percentage Composition: C 75.52%; H 13.47%; N 11.01%

>>Derivative: *N*-Me

Synonym(s): *N*,6-Dimethyl-5-hepten-2-amine, 9Cl. *N*,1,5-Trimethyl-4-hexenylamine, 9Cl. 2-Methyl-6-methylamino-2-heptene. Methylisooctenylamine. **Isometheptene**, BAN, INN. Octin. Octon. Octanil. Meptine. Methepton. Migrinil. NND 1964. Many other names

CAS Registry Number: 503-01-5

Molecular Formula: C₉H₁₉N

Molecular Weight: 141.256

Accurate Mass: 141.151749

Percentage Composition: C 76.53%; H 13.56%; N 9.92%

Use/Importance: Sympathomimetic, spasmolytic agent, used to treat migraine

Physical Description: Oil with amine odour

Melting Point: Mp 176-178°

Calculated Log P Data: Log P 2.35 (calc)

Other Data: Steam-volatile

Hazard & Toxicity: LD₅₀ (mus, orl) 134 mg/kg. LD₅₀ (mus, ipr) 42 mg/kg

Rare Chemicals Library: S37818-6

>>Derivative: *N*-Me; hydrochloride

CAS Registry Number: 6168-86-1

Physical Description: Hygroscopic powder

Melting Point: Mp 68°

>>Derivative: Tartrate

Synonym(s): Isometene. Isometh. Isomyl. Tega-Nyl. Tri-Grain

CAS Registry Number: 5984-50-9

>>Derivative: Citrate

Synonym(s): Colicon

Use/Importance: Spasmolytic

>>Derivative: Galactarate salt (2:1)

Synonym(s): **Isometheptene mucate**, USAN

CAS Registry Number: 7492-31-1

Physical Description: Cryst.

Melting Point: Mp 152°

Solubility: Sol. H₂O

References: