

CAS Registry Number: 50-48-6

C₂₀ H₂₃ N

1-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-

Molecular Weight

277.40

Melting Point (Experimental)

Value: 196.5 °C

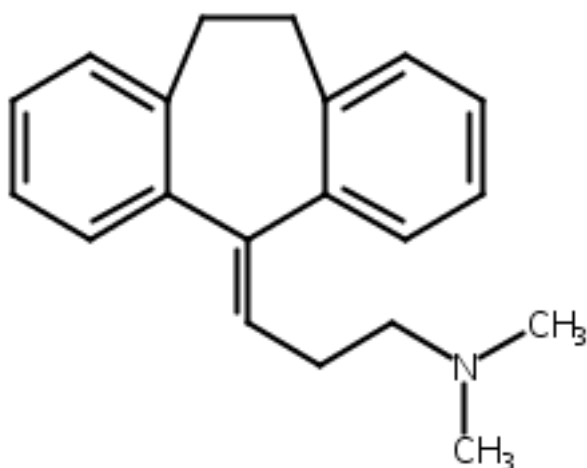
Boiling Point (Experimental)

Value: 195-205 °C

Density (Predicted)Value: 1.076±0.06 g/cm³ | Condition: Temp: 20 °C Press: 760 Torr**pKa (Predicted)**

Value: 9.18±0.28 | Condition: Most Basic Temp: 25 °C

Other Names: 5H-Dibenzo[a,d]cycloheptene-Δ⁵:γ-propylamine, 10,11-dihydro-N,N-dimethyl- (6Cl,8Cl); 3-(10,11-Dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-1-propanamine; 5-(3-Dimethylaminopropylidene)-5H-dibenzo[a,d]-10,11-dihydrocycloheptene; 5-(3'-Dimethylaminopropylidene)-dibenzo-[a,d][1,4]-cycloheptadiene; 5-(γ-Dimethylaminopropylidene)-10,11-dihydro-5H-dibenzo[a,d]cycloheptene; 5-(γ-Dimethylaminopropylidene)-5H-dibenzo(a,d)(1,4)cycloheptadiene; Adepress; Amitriprolidine; Amitriptylin; Amitriptyline; Damilen; Damitriptyline; Flavyl; MK 230; N 750; Proheptadiene; Seroten; Triptanol; Triptisol



~8996 References

~31 Commercial Sources

Experimental Properties: Biological Chemical Interface Lipinski Spectra Structure Related Thermal

Biological Properties	Value	Condition	Note
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text	1 of 11	(2)CAS
Half-Life (Biological)	See full text		(9)CAS
LC50	See full text		(11)CAS
Median Lethal Dose(LD50)	478 mg/kg	Organism: mouse Route: intraperitoneal	(15)CAS
Median Lethal Dose(LD50)	350 mg/kg	Organism: mouse Route: oral	(16)CAS
Median Lethal Dose(LD50)	86 mg/kg	Organism: mouse Route: intraperitoneal	(17)CAS
Median Lethal Dose(LD50)	38 mg/kg	Organism: mouse Route: intravenous	(18)CAS
Median Lethal Dose(LD50)	26 mg/kg	Organism: mouse Route: intravenous	(17)CAS
Chemical Properties	Value	Condition	Note
Acid/Base Dissociation Constant (K _a /K _b)	See full text	1 of 18	(1)CAS
logD	See full text	1 of 4	(2)CAS
logP	See full text	1 of 12	(12)CAS
Partition Coefficient	See full text		(24)CAS
Solubility	See full text		(2)CAS
Interface Properties	Value	Condition	Note
Surface Tension	See full text		(25)IC

Lipinski Properties	Value	Condition	Note
logP	See full text	1 of 12	(12)CAS
Structure Related Properties	Value	Condition	Note
Polar Surface Area	See full text	1 of 2	(2)CAS
Thermal Properties	Value	Condition	Note
Boiling Point	200-210 °C	Press: 5 Torr	(3)CAS
Boiling Point	195-205 °C		(4)CAS
Boiling Point	170 °C	Press: 0.9 Torr	(5)CAS
Boiling Point	170 °C	Press: 0.9 Torr	(6)CAS
Boiling Point	168-170 °C	Press: 0.6 Torr	(5)CAS
Boiling Point	164-166 °C	Press: 1 Torr	(7)CAS
Melting Point	228-230 °C		(19)CAS
Melting Point	196.5 °C		(20)SRC
Melting Point	196.0 °C		(21)CAS
Melting Point	193-194 °C	Solv: ethanol (64-17-5); ethyl ether (60-29-7)	(22)CAS
Melting Point	See full text		(23)CAS
Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See full text		(8)CAS
IR Absorption Spectrum	See spectrum		(10)BIORAD
Mass Spectrum	See spectrum		(13)BIORAD
Mass Spectrum	See spectrum		(13)BIORAD
Mass Spectrum	See spectrum		(13)BIORAD
Mass Spectrum	See spectrum		(13)BIORAD
Mass Spectrum	See full text	1 of 27	(14)CAS
Proton NMR Spectrum	See full text		(8)CAS
UV and Visible Emission/Luminescence Spectrum	See full text		(26)CAS

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REGULATORY INFORMATION :**Regulatory Synonyms**

1-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl- (DSL, NZIoC, INSQ)
amitriptyline (English, French) (EINECS, ENCS)
Amitriptylin (German) (EINECS)
amitriptilina (Spanish) (EINECS)
1-propanamina, 3 - (10,11-dihidro-5H-dibenzo [a, d] ciclohepteno-5-ilideno)-N, N-dimetil - (Spanish) (INSQ)
5H-Dibenzo[a,d]cycloheptene- Δ 5, γ -propylamine, 10,11-dihydro-N,N-dimethyl-
1-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d] cyclohepten-5-ylidene)-N,N-dimethyl-
3-(10,11-dihydro-5H-dibenzo[a,d][7]annulen-5-ylidene)-N,N-dimethylpropan-1-amine
3-(10,11-dihydrodibenzo[a,d]cyclohepten-5-ylidene)propyldimethylamine
5-(γ -Dimethylaminopropylidene)-10,11-dihydro-5H-dibenzo[a,d]cycloheptene
5-(γ -Dimethylaminopropylidene)-5H-dibenzo(a,d)(1,4)cycloheptadiene
5-(3'-Dimethylaminopropylidene)-dibenzo-[a,d][1,4]-cycloheptadiene
5-(3-Dimethylaminopropylidene)-5H-dibenzo[a,d]-10,11-dihydrocycloheptene
Adepress
Amitriprolidine
Amitriptylin (English, Danish, Swedish)
Damilen
Damitriptyline
Flavyl
MK 230
N 750
Proheptadiene
Seroten
Triptanol
Triptisol
3-(10,11-dihydrodibenzo[a,d]cycloheptene-5-ylidene)propyldimethylamine (French)
3-(10,11-Dihydrodibenzo[a,d]cyclohepten-5-yliden)propyldimethylamin (German, Danish)
3-(10,11-dihidro-dibenzo[a,d]ciclohepten-5-iliden)propildimetilamina (Spanish)
3-(10,11-diidro-dibenzo[a,d]ciclohepten-5-iliden)propildimetilamina (Italian)
amitriptilina (Italian, Portuguese)
3-(10,11-dihydrodibenzo[a,d]cyclohepteen-5-ylideen)propyldimethylamine (Dutch)
amitriptyline (Dutch)
3-(10,11-dihydrodibentso[a,d]syklohepten-5-ylideeni)propyylidimetyyliamiini (Finnish)

amitriptyliini (Finnish)

3-(10,11-dihydrodibenzo[a,d]ciclohepteno-5-ilideno)propildimetilamina (Portuguese)

3-(10,11-dihydrodibenso[a,d]cyklohepten-5-yliden)propyldimetylamin (Swedish)

Regulatory Overview by Country

Confidentiality Status

Public

Canada

Inventory Status

On DSL

Canada Gazette, Part II, February 11, 2004

European Union

EU Customs Code CN:

29214900

Inventory Status

On REACH

REACH: List of Registered Substances, 2018 <https://echa.europa.eu/substance-information/-/substanceinfo/100.000.038>

On EINECS

Annex to Official Journal of the European Communities, 15 June 1990

Regulatory List Number

EC No.: 200-041-6

EINECS No.: 200-041-6

Japan

Inventory Status

On ENCS

Japanese Gazette

Contained within class: Low Molecular Carbo-polycyclic Organic Compounds.

Regulatory List Number

ENCS No.: 9-57

Mexico

Inventory Status

On INSQ

National Inventory of Chemical Substances in Mexico, 2012

New Zealand

Inventory Status

On NZIoC

New Zealand Inventory of Chemicals, 2006

May be used as a component in a product covered by a group standard but it is not approved for use as a chemical in its

own right.

International and other lists

Harmonized Tariff Code

292149

Regulatory Inventories

====European Community Regulations====

European Community Legislation

Official Journal of the European Union, No L 342 #52:59 (22 Dec 2009).

Commission Regulation (EC) No 1223/2009 of the European Parliament and of the Council on 30 November 2009 concerning cosmetic products. This substance is included in Annex II, List of Substances Prohibited in Cosmetic Products.

====Canadian Regulations====

Canadian Legislation Affecting Chemicals

Canada Gazette, Part I, 150 #6:152 (06 Feb 2016).

The Chemicals Management Plan (CMP) is a Government of Canada initiative aimed at reducing risks posed by chemicals to Canadians and their environment. Environment and Climate Change Canada and Health Canada are inviting stakeholders to provide information that will inform the path forward for the next phase of the CMP. This substance has been identified as requiring human health and ecological assessments.

File Segment

CANADA: DSL

EEC: EINECS

EU: REACH

Harmonized Tariff Code: HTC

JAPAN: ENCS

MEXICO: INSQ

NEW ZEALAND: NZIoC

Bioactivity Indicators	References
Antidiabetic agents (all) > Antidiabetic agents	131
Anti-infective agents (all) >>> Antibacterial agents	68
Anti-infective agents (all) >>> Antibiotics	135
Anti-infective agents (all) >>> Antiviral agents	100
Anti-infective agents (all) >>> Fungicides	96
Anti-inflammatory agents (all) > Anti-inflammatory agents	260
Anti-inflammatory agents (all) > Antirheumatic agents	58
Anti-inflammatory agents (all) > Nonsteroidal anti-inflammatory agents	239
Antitumor agents (all) > Antitumor agents	235
Cardiovascular agents (all) >> Antiarrhythmics	106
Cardiovascular agents (all) >> Antihypertensives	126
Cardiovascular agents (all) > Cardiovascular agents	94
Cytoprotective agents (all) > Neuroprotective agents	126
Enzyme inhibitors (all) > Monoamine oxidase inhibitors	130
Gastrointestinal agents (all) > Antiemetics	86
Gastrointestinal agents (all) > Gastrointestinal agents	51
Hematologic agents (all) >>> Anticoagulants	68

Membrane transport modulators (all) >>> Calcium channel blockers	136
Membrane transport modulators (all) >> Sodium channel blockers	64
Nervous system agents (all) >>>> β -Adrenoceptor antagonists	134
Nervous system agents (all) >>> Analgesics	674
Nervous system agents (all) >>> Anesthetics	85
Nervous system agents (all) >>> Anti-Alzheimer agents	105
Nervous system agents (all) >> Anticonvulsants	405
Nervous system agents (all) >> Anticonvulsants	405
Nervous system agents (all) >>>> Antidepressants	1546
Nervous system agents (all) >> Antiemetics	86
Nervous system agents (all) >>> Antimigraine agents	120
Nervous system agents (all) >>> Antiobesity agents	58
Nervous system agents (all) >> Antiparkinsonian agents	147
Nervous system agents (all) >>>> Antipsychotics	491
Nervous system agents (all) >>>> Antipsychotics	491
Nervous system agents (all) >> Anxiolytics	312
Nervous system agents (all) >> Central nervous system agents	112
Nervous system agents (all) >> Central nervous system stimulants	56
Nervous system agents (all) >>> Cholinergic antagonists	116
Nervous system agents (all) >>> Cognition enhancers	68
Nervous system agents (all) >>> Dopamine agonists	54
Nervous system agents (all) >>> 5-HT agonists	65
Nervous system agents (all) >>> 5-HT antagonists	80
Nervous system agents (all) >> 5-HT reuptake inhibitors	505
Nervous system agents (all) >>> Hypnotics and Sedatives	190
Nervous system agents (all) >>> Hypnotics and Sedatives	190
Nervous system agents (all) >>> Local anesthetics	87
Nervous system agents (all) >> Mood stabilizers	67
Nervous system agents (all) > Nervous system agents	107
Nervous system agents (all) > Neuroprotective agents	126
Nervous system agents (all) >>> NMDA receptor antagonists	85
Nervous system agents (all) >> Noradrenaline reuptake inhibitors	142
Nervous system agents (all) >>>> Opioids	277
Nervous system agents (all) >>> Psychotropics	158
Nervous system agents (all) >> Serotonin-noradrenaline reuptake inhibitors	172
Nervous system agents (all) >>>> Tranquilizers	95
Nervous system agents (all) >>> Tranquilizers	95
Nervous system agents (all) >>>> Tricyclic antidepressants	654
Neuromuscular agents (all) >> Muscle relaxants	99
Pharmaceutical immune agents (all) >> Allergy inhibitors	51
Pharmaceutical immune agents (all) >> Immunomodulators	64
Pharmaceutical immune agents (all) >>> Immunosuppressants	82
Receptor agonists (all) >>> Dopamine agonists	54
Receptor agonists (all) >>> 5-HT agonists	65
Receptor antagonists (all) >>>> β -Adrenoceptor antagonists	134
Receptor antagonists (all) >> Antihistamines	160
Receptor antagonists (all) >>> Cholinergic antagonists	116
Receptor antagonists (all) >> Histamine H1 receptor antagonists	50
Receptor antagonists (all) >>> 5-HT antagonists	80
Receptor antagonists (all) >>> NMDA receptor antagonists	85
Renal agents (all) >> Diuretics	73
Respiratory system agents (all) > Antiasthmatics	66

Document Type(s): Conference, Dissertation, Journal, Patent, Preprint, Report

Source of Registration: CA