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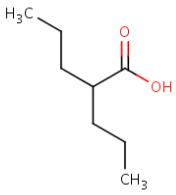
ChemIDplus
A TOXNET DATABASE

Start New Query | Modify Query | Search History | Show Query | Switch to Summary View

Substance Name: Valproic acid [USAN:USP:INN:BAN]
RN: 99-66-1
InChIKey: NIJJYAXOARWZEE-UHFFFAOYSA-N



Note
A fatty acid with anticonvulsant properties used in the treatment of epilepsy. The mechanisms of its therapeutic actions are not well understood. It may act by increasing GAMMA-AMINOBUTYRIC ACID levels in the brain or by altering the properties of voltage dependent sodium channels.

Molecular Formula
C8-H16-O2

Molecular Weight
144.2124

All | Classifications | Links to Resources | Names & Synonyms | Registry Numbers | Structure Descriptors | Toxicity | Physical Properties

Classification Codes

- Anticonvulsant
- Anticonvulsants
- Antimanic agents
- Central Nervous System Agents
- Central Nervous System Depressants
- Drug / Therapeutic Agent
- Enzyme inhibitors
- GABA agents
- Human Data
- Neurotransmitter Agents
- Psychotropic Drugs
- Reproductive Effect
- Tranquilizing Agents

Links to Resources

NLM Resources (File Locators)

- ClinicalTrials.gov
- DailyMed
- DrugPortal
- EMIC
- HSDB
- MedlinePlusDrug
- MeSH
- PubChem
- PubMed
- PubMed AIDS
- PubMed Cancer
- PubMed Toxicology
- RTECS
- TOXLINE
- Pillbox
- PubMed Health
- LactMed
- MedlinePlusAll

Other Resources (Internet Locators)

- DrugDigest
- Drugs@FDA
- NIAID ChemDB
- NIST WebBook
- USA.gov
- EPA ACToR

Search for this InChIKey on the Web

Names and Synonyms

Name of Substance

- Valproic acid
- Valproic acid [USAN:USP:INN:BAN]

MeSH Heading

- Valproic acid

Synonyms

- 2-Propylpentanoic acid
- 2-Propylvaleric acid
- 3-02-00-00807 (Beilstein Handbook Reference)
- 4-Heptanecarboxylic acid
- 44089
- Abbott 44090
- Acetic acid, dipropyl-
- Acide valproique
- Acide valproique [INN-French]
- Acido valproico
- Acido valproico [INN-Spanish]
- Acidum valproicum
- Acidum valproicum [INN-Latin]
- AI3-10500
- BRN 1750447
- Depakene
- Depakin
- Depakine
- Di-n-propylacetic acid
- Di-n-propylessigsaure
- Di-n-propylessigsaure [German]
- Dipropylacetate
- Dipropylacetic acid
- DPA (VAN)
- EINECS 202-777-3
- Ergenyl
- HSDB 3582
- Kyselina 2-propylvalerova
- Kyselina 2-propylvalerova [Czech]
- Mylproin
- Myproic acid
- n-Dipropylacetic acid
- NSC 93819
- Propylvaleric acid
- Stavzor
- UNII-614OI1Z5WI
- Valproate
- Valproic acid
- Vupral

Systematic Names

- 2-Propylvaleric acid
- Pentanoic acid, 2-propyl-
- Valeric acid, 2-propyl-

Superlist Names

- Valproate
- Valproic acid

Registry Numbers

CAS Registry Number

- 99-66-1

Related Registry Number

- 76584-70-8 (hydrochloride salt (2:1))

System Generated Number

- 0000099661

Structure Descriptors

InChI

1S/C8H16O2/c1-3-5-7(6-4-2)8(9)10/h7H,3-6H2,1-2H3,(H,9,10)

Download

http://chem.sis.nlm.nih.gov/chemidplus/rn/99-66-1

InChI

1S/C8H16O2/c1-3-5-7(6-4-2)8(9)10/h7H,3-6H2,1-2H3,(H,9,10)

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InChIKey

NIJJYAXOARWZEE-UHFFFAOYSA-N

Search the web for this InChIKey

Smiles

C(CCC)(CCC)C(O)=O

Download

Toxicity

Organism	Test Type	Route	Reported Dose (Normalized Dose)	Effect	Source
child	TDLo	oral	375mg/kg (375mg/kg)	CARDIAC: PULSE RATE INCREASE WITHOUT FALL IN BP LUNGS, THORAX, OR RESPIRATION: CYANOSIS VASCULAR: BP LOWERING NOT CHARACTERIZED IN AUTONOMIC SECTION	Critical Care Medicine. Vol. 21, Pg. 299, 1993. Link to PubMed
child	TDLo	oral	412mg/kg (412mg/kg)	LUNGS, THORAX, OR RESPIRATION: DYSPNEA CARDIAC: PULSE RATE INCREASE WITHOUT FALL IN BP BEHAVIORAL: COMA	Journal of Analytical Toxicology. Vol. 20, Pg. 55, 1996. Link to PubMed
child	TDLo	oral	10500mg/kg/30 (10500mg/kg)	GASTROINTESTINAL: CHANGES IN STRUCTURE OR FUNCTION OF ENDOCRINE PANCREAS GASTROINTESTINAL: NAUSEA OR VOMITING	American Journal of Diseases of Children. Vol. 138, Pg. 912, 1984. Link to PubMed
child	TDLo	unreported	1800mg/kg/60D (1800mg/kg)	GASTROINTESTINAL: NAUSEA OR VOMITING GASTROINTESTINAL: CHANGES IN STRUCTURE OR FUNCTION OF ENDOCRINE PANCREAS	Lancet. Vol. 1, Pg. 1196, 1980.
guinea pig	LD50	oral	824mg/kg (824mg/kg)		"Pharmacodynamie de l'Acide Dipropylacetique Vol. -, Pg. 39, 1968.
human	TDLo	oral	13333ug/kg/D-I (13.333mg/kg)	BEHAVIORAL: SLEEP	New England Journal of Medicine. Vol. 301, Pg. 435, 1979.
man	LDLo	oral	736mg/kg (736mg/kg)	LUNGS, THORAX, OR RESPIRATION: ACUTE PULMONARY EDEMA BRAIN AND COVERINGS: OTHER DEGENERATIVE CHANGES	Journal of Analytical Toxicology. Vol. 22, Pg. 537, 1998. Link to PubMed
man	TDLo	oral	21mg/kg/2D-I (21mg/kg)	BEHAVIORAL: SOMNOLENCE (GENERAL DEPRESSED ACTIVITY)	Neurology. Vol. 37, Pg. 886, 1987. Link to PubMed
man	TDLo	oral	429mg/kg (429mg/kg)	BEHAVIORAL: COMA	Journal of Toxicology, Clinical Toxicology. Vol. 38, Pg. 219, 2000.
mouse	LD50	intraperitoneal	470mg/kg (470mg/kg)		Chimica Therapeutica. Vol. 3, Pg. 430, 1968.
mouse	LD50	oral	1098mg/kg (1098mg/kg)		European Patent Application. Vol. #78785,
mouse	LD50	subcutaneous	860mg/kg (860mg/kg)		"Pharmacodynamie de l'Acide Dipropylacetique Vol. -, Pg. 38, 1968.
rabbit	LD50	intraperitoneal	1200mg/kg (1200mg/kg)		"Pharmacodynamie de l'Acide Dipropylacetique Vol. -, Pg. 39, 1968.
rat	LD50	oral	670mg/kg (670mg/kg)	BEHAVIORAL: SOMNOLENCE (GENERAL DEPRESSED ACTIVITY) GASTROINTESTINAL: "HYPERMOTILITY, DIARRHEA"	Food and Cosmetics Toxicology. Vol. 2, Pg. 327, 1964.
women	TDLo	oral	100mg/kg/10D-I (100mg/kg)	BEHAVIORAL: GENERAL ANESTHETIC BRAIN AND COVERINGS: ENCEPHALITIS BRAIN AND COVERINGS: CHANGES IN SURFACE EEG	Journal of Toxicology, Clinical Toxicology. Vol. 38, Pg. 219, 2000.
women	TDLo	oral	330mg/kg (330mg/kg)	BEHAVIORAL: COMA BRAIN AND COVERINGS: CHANGES IN SURFACE EEG LUNGS, THORAX, OR RESPIRATION: OTHER CHANGES	American Journal of Emergency Medicine. Vol. 18, Pg. 508, 2000. Link to PubMed

Physical Properties

Physical Property	Value	Units	Temp (deg C)	Source
Boiling Point	222	deg C		EXP
pKa Dissociation Constant	4.6	(none)		EXP
log P (octanol-water)	2.75	(none)		EXP
Water Solubility	2000	mg/L	20	EXP
Vapor Pressure	0.046	mm Hg	25	EST
Henry's Law Constant	3.00E-06	atm-m3/mole	25	EST
Atmospheric OH Rate Constant	8.18E-12	cm3/molecule-sec	25	EST

Physical property data is provided to ChemIDplus by Syracuse Research Corporation.

See all available property data for this compound, including references.

http://chem.sis.nlm.nih.gov/chemidplus/rn/99-66-1

Atmospheric OH Rate Constant	8.18E-12	cm3/molecule-sec	25	EST

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