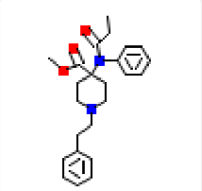
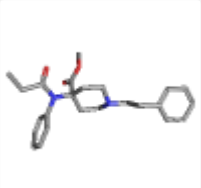
PubChem

COMPOUND SUMMARY

# Carfentanil

| | |
|---|---|
| **PubChem CID** | 62156 |
| **Structure** |  2D  3D<br>Find Similar Structures |
| **Molecular Formula** | $C_{24}H_{30}N_2O_3$ |
| **Synonyms** | CARFENTANIL<br>Carfentanyl<br>Carfentanila<br>Carfentanilum<br>Wildnil<br>More... |
| **Molecular Weight** | 394.5 |
| **Dates** | Modify 2021-09-25 Create 2005-03-28 |

Carfentanil is a DEA Schedule II controlled substance. Substances in the DEA Schedule II have a high potential for abuse which may lead to severe psychological or physical dependence.

▸ Drug Enforcement Administration (DEA)

Carfentanil is a monocarboxylic acid amide resulting from the formal condensation of the aryl amino group of methyl 4-anilino-1-(2-phenylethyl)piperidine-4-carboxylate with propanoic acid. It has a role as a mu-opioid receptor agonist, an opioid analgesic and a tranquilizing drug. It is a member of piperidines, a methyl ester, a tertiary amino compound and a tertiary carboxamide.

▸ ChEBI

Carfentanil or carfentanyl (Wildnil) is an analogue of the popular synthetic opioid analgesic fentanyl, and is one of the most potent opioids known (also the most potent opioid used commercially). Carfentanil was first synthesized in 1974 by a team of chemists at Janssen Pharmaceutica which included Paul Janssen. It has a quantitative potency approximately 10,000 times that of morphine and 100 times that of fentanyl, with activity in humans starting at about 1 microgram. It is marketed under the trade name Wildnil as a general anaesthetic agent for large animals. Carfentanil is intended for large-animal use only as its extreme potency makes it inappropriate for use in humans. Currently sufentanil, approximately 10–20

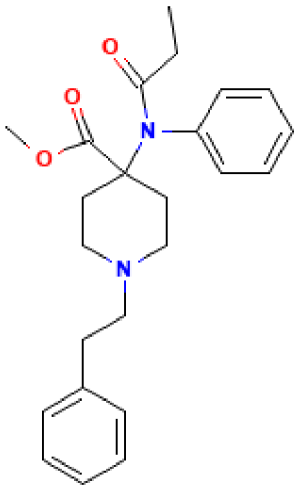
times less potent (500 to 1000 times the efficacy of **morphine** per weight) than carfentanil, is the maximum strength **fentanyl** analog for use in humans.

- **DrugBank**

# 1 Structures

## 1.1 2D Structure

Chemical Structure Depiction

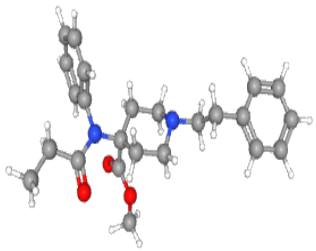



PubChem

## 1.2 3D Conformer

Interactive Chemical Structure Model

- (•) Ball and Stick
- ( ) Sticks
- ( ) Wire-Frame
- ( ) Space-Filling
- [x] Show Hydrogens
- [ ] Animate



PubChem

# 2 Names and Identifiers

## 2.1 Computed Descriptors

### 2.1.1 IUPAC Name

methyl 1-(2-phenylethyl)-4-(*N*-propanoylanilino)piperidine-4-carboxylate

*Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)*

PubChem

### 2.1.2 InChI

InChI=1S/C24H30N2O3/c1-3-22(27)26(21-12-8-5-9-13-21)24(23(28)29-2)15-18-25(19-16-24)17-14-20-10-6-4-7-11-20/h4-13H,3,14-19H2,1-2H3

*Computed by InChI 1.0.6 (PubChem release 2021.05.07)*

PubChem

### 2.1.3 InChI Key

YDSDEBIZUNNPOB-UHFFFAOYSA-N

*Computed by InChI 1.0.6 (PubChem release 2021.05.07)*

PubChem

### 2.1.4 Canonical SMILES

CCC(=O)N(C1=CC=CC=C1)C2(CCN(CC2)CCC3=CC=CC=C3)C(=O)OC

*Computed by OEChem 2.3.0 (PubChem release 2021.05.07)*

PubChem

## 2.2 Molecular Formula

C24H30N2O3

*Computed by PubChem 2.1 (PubChem release 2021.05.07)*

PubChem

## 2.3 Other Identifiers

### 2.3.1 CAS

59708-52-0

CAS Common Chemistry; ChemIDplus; DrugBank; EPA DSSTox; Hazardous Substances Data Bank (HSDB)

### 2.3.2 Related CAS

61380-27-6 (citrate)

- ChemIDplus

### 2.3.3 Deprecated CAS

60645-15-0

- ChemIDplus

### 2.3.4 UNII

LA9DTA2L8F

- FDA/SPL Indexing Data

### 2.3.5 DEA Code Number

9743

- Drug Enforcement Administration (DEA)

### 2.3.6 DSSTox Substance ID

DTXSID40208427

- EPA DSSTox

### 2.3.7 Wikipedia

Carfentanil

- Wikipedia

## 2.4 Synonyms

### 2.4.1 MeSH Entry Terms

(4-methoxycarbonyl)fentanyl
11C-carfentanil
4-methoxycarbonyl fentanyl
4-methoxycarbonylfentanyl
carfentanil
carfentanil citrate
carfentanil oxalate
carfentanil, (+-)-isomer
carfentanyl
R 31833
R 33799
R-31833
R31833

Medical Subject Headings (MeSH)

## 2.4.2 Depositor-Supplied Synonyms

| | |
|---|---|
| CARFENTANIL | 4-((1-Oxopropyl)phenylamino)-1-(2-phenylethyl)-4 |
| Carfentanyl | LA9DTA2L8F |
| Carfentanila | R-33799 |
| Carfentanilum | CHEMBL290429 |
| Wildnil | R-31833 |
| 59708-52-0 | Carfentanil (INN) |
| Carfentanil [INN] | Carfentanila [Spanish] |
| UNII-LA9DTA2L8F | methyl 1-(2-phenylethyl)-4-[phenyl(propionyl)amir |
| Methyl 1-phenylethyl-4-(N-phenylpropionamido)isonipecotate | Carfentanilum [INN-Latin] |
| CHEBI:61084 | Carfentanila [INN-Spanish] |
| Methyl 4-(N-(1-oxopropyl)-N-phenylamino)-1-(2-phenylethyl)-4-piperidinecarboxylate | (4-methoxycarbonyl)fentanyl |
| Methyl 4-(N-propionyl-N-phenylamino)-1-(2-phenylethyl)-4-piperidine-carboxylate | BRN 0456976 |

PubChem

# 3 Chemical and Physical Properties

## 3.1 Computed Properties

| Property Name | Property Value | Reference |
|---|---|---|
| Molecular Weight | 394.5 | Computed by PubChem 2.1 (PubChem release 2021.05.07) |
| XLogP3 | 3.8 | Computed by XLogP3 3.0 (PubChem release 2021.05.07) |
| Hydrogen Bond Donor Count | 0 | Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07) |
| Hydrogen Bond Acceptor Count | 4 | Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07) |
| Rotatable Bond Count | 8 | Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07) |
| Exact Mass | 394.22564282 | Computed by PubChem 2.1 (PubChem release 2021.05.07) |
| Monoisotopic Mass | 394.22564282 | Computed by PubChem 2.1 (PubChem release 2021.05.07) |
| Topological Polar Surface Area | 49.8 Å$^2$ | Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07) |
| Heavy Atom Count | 29 | Computed by PubChem |
| Formal Charge | 0 | Computed by PubChem |
| Complexity | 530 | Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07) |
| Isotope Atom Count | 0 | Computed by PubChem |
| Defined Atom Stereocenter Count | 0 | Computed by PubChem |
| Undefined Atom Stereocenter Count | 0 | Computed by PubChem |
| Defined Bond Stereocenter Count | 0 | Computed by PubChem |
| Undefined Bond Stereocenter Count | 0 | Computed by PubChem |
| Covalently-Bonded Unit Count | 1 | Computed by PubChem |
| Compound Is Canonicalized | Yes | Computed by PubChem (release 2021.05.07) |

PubChem

## 3.2 Experimental Properties

### 3.2.1 Solubility

In water, 4.21 mg/L at 25 °C (est)

*US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of May 11, 2017:* ***https://www2.epa.gov/tsca-screening-tools***

Hazardous Substances Data Bank (HSDB)

### 3.2.2 Vapor Pressure

2.03X10-10 mm Hg at 25 °C (est)

*US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of May 11, 2017:* ***https://www2.epa.gov/tsca-screening-tools***

Hazardous Substances Data Bank (HSDB)

### 3.2.3 LogP

log Kow = 3.39 (est)

*US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of May 11, 2017:* ***https://www2.epa.gov/tsca-screening-tools***

▶ **Hazardous Substances Data Bank (HSDB)**

## 3.2.4 Henrys Law Constant

Henry's Law constant = of 4.37X10-13 atm-cu m/mole at 25 °C (est)

*US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of May 11, 2017:* ***https://www2.epa.gov/tsca-screening-tools***

▶ **Hazardous Substances Data Bank (HSDB)**

## 3.2.5 Dissociation Constants

pKa = 8.05 (est)

***PMID:16381955***

*Full text:* ***https://www.ncbi.nlm.nih.gov/pmc/articles/PMC1347430***

*Wishart DS et al; Nucleic Acids Res 34: D668-72 (2006). Available from, as of May 11, 2017:* ***https://www.drugbank.ca/***

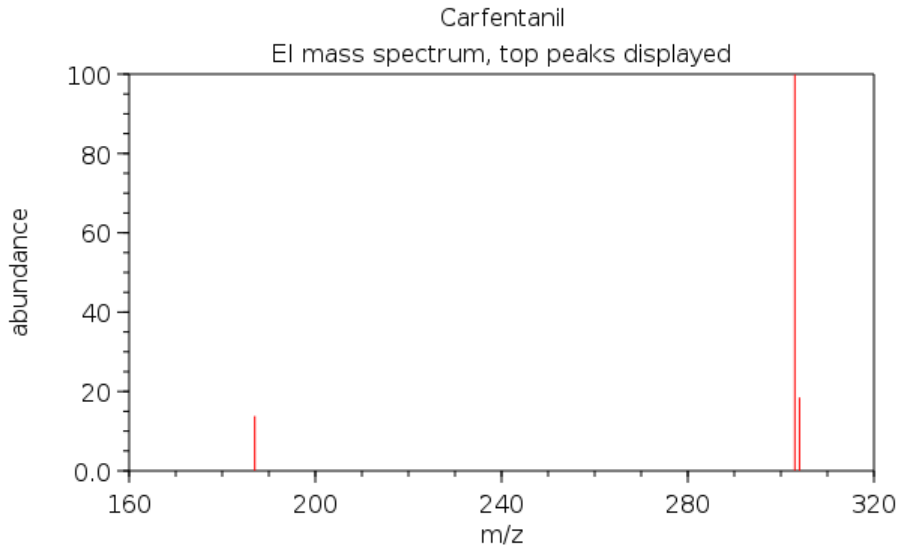
▶ **Hazardous Substances Data Bank (HSDB)**

# 4 Spectral Information

## 4.1 Mass Spectrometry

### 4.1.1 GC-MS

Showing 2 of 10 View More

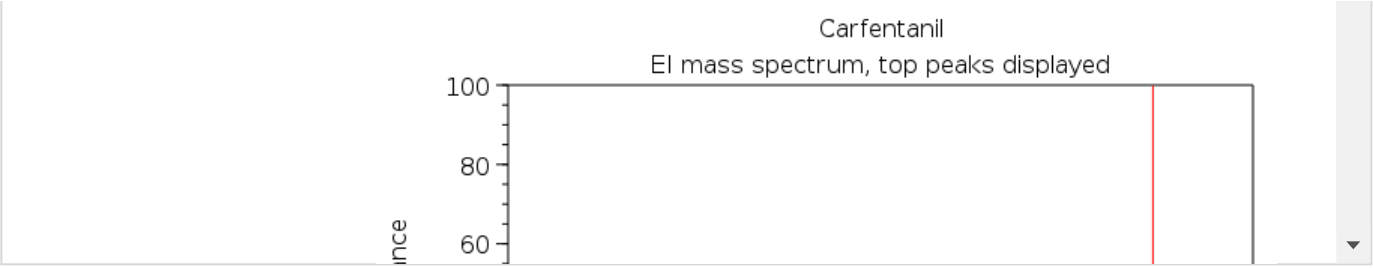
| | |
|---|---|
| **NIST Number** | 248193 |
| **Library** | Main library |
| **Total Peaks** | 151 |
| **m/z Top Peak** | 303 |
| **m/z 2nd Highest** | 304 |
| **m/z 3rd Highest** | 187 |
| **Thumbnail** |  |





NIST Mass Spectrometry Data Center

| | |
|---|---|
| **NIST Number** | 120336 |
| **Library** | Replicate library |
| **Total Peaks** | 43 |
| **m/z Top Peak** | 303 |
| **m/z 2nd Highest** | 42 |
| **m/z 3rd Highest** | 105 |
| **Thumbnail** | |



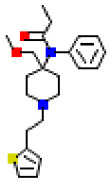
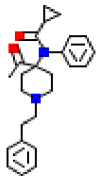
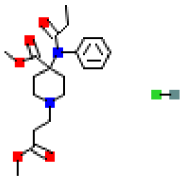
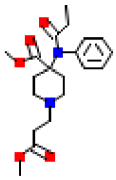
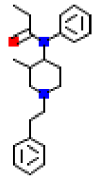

NIST Mass Spectrometry Data Center

# 5 Related Records

## 5.1 Related Compounds with Annotation

401 items View More Rows & Details

SORT BY Compound CID

| Structure | Compound CID | Name | Molecular Formula | Molecular Weight, g/mol |
|---|---|---|---|---|
|  | 41693 | Sufentanil | $C_{22}H_{30}N_2O_2S$ | 386.6 |
|  | 43381 | Cyclopropanecarboxamide, N-(4-acetyl-1-(2-phenylethyl)-4-piperidinyl)-N-phenyl- | $C_{25}H_{30}N_2O_2$ | 390.5 |
|  | 60814 | Remifentanil hydrochloride | $C_{20}H_{29}ClN_2O_5$ | 412.9 |
|  | 60815 | Remifentanil | $C_{20}H_{28}N_2O_5$ | 376.4 |
|  | 61996 | Mefentanyl | $C_{23}H_{30}N_2O$ | 350.5 |

1 2 3 ... 81 Next

PubChem

## 5.2 Related Compounds

| | |
|---|---|
| Same Connectivity | 5 Records |
| Same Parent, Connectivity | 12 Records |
| Same Parent, Exact | 7 Records |
| Mixtures, Components, and | 12 Records |

| | |
|---|---|
| Neutralized Forms | |
| Similar Compounds | 241 Records |
| Similar Conformers | 209 Records |

PubChem

## 5.3 Substances

### 5.3.1 Related Substances

| | |
|---|---|
| All | 83 Records |
| Same | 46 Records |
| Mixture | 37 Records |

PubChem

### 5.3.2 Substances by Category

PubChem

## 5.4 Entrez Crosslinks

| | |
|---|---|
| PubMed | 71 Records |
| Taxonomy | 2 Records |
| Gene | 16 Records |

PubChem

## 5.5 Associated Chemicals

Carfentanil citrate; 61380-27-6

Hazardous Substances Data Bank (HSDB)

## 5.6 NCBI LinkOut

- NCBI

# 6 Chemical Vendors

- PubChem

# 7 Drug and Medication Information

## 7.1 Drug Indication

Carfentanil is similar (but more potent) to the opioid analgesic **fentanyl**. It is used as a tranquilizer for large animals.

▶ DrugBank

## 7.2 Clinical Trials

### 7.2.1 ClinicalTrials.gov

▶ ClinicalTrials.gov

## 7.3 DEA Controlled Substances

| | |
|---|---|
| **Substance** | Carfentanil |
| **Synonym(s)** | Wildnil |
| **DEA Controlled Substances Code Number** | 9743 |
| **Controlled Substances Act Schedule** | Schedule II - Substances in the DEA Schedule II have a high potential for abuse which may lead to severe psychological or physical dependence. |
| **Narcotic** | Yes |

▶ Drug Enforcement Administration (DEA)

## 7.4 Therapeutic Uses

Analgesics, Opioid

*National Library of Medicine's Medical Subject Headings. Carfentanil. Online file (MeSH, 2017). Available from, as of April 26, 2017: **https://www.nlm.nih.gov/mesh/2017/mesh_browser/MBrowser.html***

▶ Hazardous Substances Data Bank (HSDB)

VET: Large animal immobilizing agent use in Cervidae (Deer, elk, moose) /**Carfentanil citrate**/

*US FDA; Freedom of Information Act (FOIA) Drug Summaries. Wildnil. NADA 139-633. Available from, as of May 11, 2017:*
***https://www.fda.gov/downloads/AnimalVeterinary/Products/ApprovedAnimalDrugProducts/FOIADrugSummaries/UCM473748.pdf***

▶ **Hazardous Substances Data Bank (HSDB)**

VET: Safe anesthesia of zoo animals is of special concern. Many procedures routinely accomplished on domestic animals with minimal restraint require anesthesia of zoologic species for the welfare and safety of both zoo animals and personnel. ... The potent opioids **etorphine**, carfentanil, and **thiofentanil**, alone or in combination with other agents (eg, azaparone, **acepromazine**, **xylazine**, **detomidine**), have been used extensively for anesthesia of ungulates, elephants, and rhinoceros.

*Kahn, C.M (ed.).; The Merck Veterinary Manual 10th Edition. Merck & Co. Whitehouse Station NJ. 2010, p. 1814-5*

▶ **Hazardous Substances Data Bank (HSDB)**

VET: October 2001 to January 2002, captive free-ranging white-tailed deer (Odocoileus virginianus) were immobilized with a combination of **carfentanil citrate** and **xylazine hydrochloride**. From this study, we selected a dose of carfentanil/**xylazine** for the purpose of comparing immobilization parameters and physiologic effects with those of a combination of **tiletamine** and **zolazepam** (Telazol) and **xylazine**. Animals were initially given intramuscular injections of 10 mg **xylazine** and one of four doses of carfentanil (i.e., 0.5, 1.0, 1.5, and 2.0 mg). A carfentanil dose of 1.2 mg (x +/- SD = 23.5 +/- 3.2 microg/kg) and 10 mg **xylazine** (0.2 +/- 0.03 mg/kg) were selected, based on induction times and previously published reports, to compare with a combination of 230 mg of Telazol (4.5 +/- 0.6 mg/kg) and 120 mg **xylazine** (2.3 +/- 0.3 mg/kg). Time to first observable drug effects and to induction were significantly longer for deer treated with carfentanil/**xylazine** than with Telazol/**xylazine** ($P < 0.01$). Hyperthermia was common in deer immobilized with carfentanil/xylazine, but heart rate, respiration rate, and hemoglobin saturation were within acceptable levels. Degree of anesthesia of deer immobilized with Telazol/xylazine was superior to deer immobilized with carfentanil/xylazine. The combination of 120 mg of naltrexone hydrochloride and 6.5 mg of yohimbine hydrochloride provided rapid and complete reversal (1.9 +/- 1.1 min) of carfentanil/xylazine immobilization. Animals immobilized with Telazol/xylazine had long recovery times with occasional resedation after antagonism with 6.5 mg of yohimbine. The combination of carfentanil and xylazine at the doses tested did not provide reliable induction or immobilization of white-tailed deer even though drug reversal was rapid and safe using naltrexone and yohimbine.

***PMID:14733280***
*Miller BF et al; J Wildl Dis 39 (4): 851-8 (2003)*

▶ **Hazardous Substances Data Bank (HSDB)**

For more Therapeutic Uses (Complete) data for Carfentanil (8 total), please visit the **HSDB record page**.

▶ **Hazardous Substances Data Bank (HSDB)**

# 8 Pharmacology and Biochemistry

## 8.1 Pharmacology

Carfentanil acts primarily on the mu (some kappa and delta) opioid receptors as an agonist. It will induce similar effects of analgesia as other opioids, however, due to its potency, it will also induce strong side effects such as sedation. Consequently, that is why it is used as a tranquilizer for large animals. Carfentanil interacts predominately with the opioid mu-receptor. These mu-binding sites are discretely distributed in the brain, spinal cord, and other tissues. It exerts its principal pharmacologic effects on the central nervous system. Its primary actions of therapeutic value are analgesia and sedation. Carfentanil also depresses the respiratory centers, depresses the cough reflex, and constricts the pupils.

▸ DrugBank

## 8.2 MeSH Pharmacological Classification

**Analgesics, Opioid**

Compounds with activity like OPIATE ALKALOIDS, acting at OPIOID RECEPTORS. Properties include induction of ANALGESIA or NARCOSIS. (See **all compounds classified as Analgesics, Opioid**.)

▸ Medical Subject Headings (MeSH)

## 8.3 Metabolism/Metabolites

Carfentanil is an ultra-potent synthetic opioid. No human carfentanil metabolism data are available. Reportedly, Russian police forces used carfentanil and **remifentanil** to resolve a hostage situation in Moscow in 2002. This alleged use prompted interest in the pharmacology and toxicology of carfentanil in humans. Our study was conducted to identify human carfentanil metabolites and to assess carfentanil's metabolic clearance, which could contribute to its acute toxicity in humans. We used Simulations Plus's ADMET Predictor and Molecular Discovery's MetaSite to predict possible metabolite formation. Both programs gave similar results that were generally good but did not capture all metabolites seen in vitro. We incubated carfentanil with human hepatocytes for up to 1 hr and analyzed samples on a Sciex 3200 QTRAP mass spectrometer to measure parent compound depletion and extrapolated that to represent intrinsic clearance. Pooled primary human hepatocytes were then incubated with carfentanil up to 6 h and analyzed for metabolite identification on a Sciex 5600+ TripleTOF (QTOF) high-resolution mass spectrometer. MS and MS/MS analyses elucidated the structures of the most abundant metabolites. Twelve metabolites were identified in total. N-Dealkylation and monohydroxylation of the **piperidine** ring were the dominant metabolic pathways. Two N-oxide metabolites and one glucuronide metabolite were observed. Surprisingly, ester hydrolysis was not a major metabolic pathway for carfentanil. While the human liver microsomal system demonstrated rapid clearance by CYP enzymes, the hepatocyte incubations showed much slower clearance, possibly providing some insight into the long duration of carfentanil's effects.

*PMID:27495118*
*Feasel MG et al; AAPS J 18 (6): 1489-1499 (2016)*

▸ Hazardous Substances Data Bank (HSDB)

## 8.4 Mechanism of Action

Carfentanil binds very strongly to mu opioid receptors and acts as a competitive agonist. Opiate receptors are coupled with G-protein receptors and function as both positive and negative regulators of synaptic transmission via G-proteins that activate effector proteins. Binding of the opiate stimulates the exchange of **GTP** for GDP on the G-protein complex. As the effector system is **adenylate** cyclase and **cAMP** located at the inner surface of the plasma membrane, opioids decrease intracellular **cAMP** by inhibiting **adenylate** cyclase. Subsequently, the release of nociceptive neurotransmitters such as **substance P**, **GABA**, **dopamine**, **acetylcholine** and **noradrenaline** is inhibited. Opioids also inhibit the release of vasopressin, **somatostatin**, insulin

and **glucagon**. Opioids close N-type voltage-operated **calcium** channels (OP2-receptor agonist) and open **calcium**-dependent inwardly rectifying **potassium** channels (OP3 and OP1 receptor agonist). This results in hyperpolarization and reduced neuronal excitability.

**DrugBank**

The positron emission tomography (PET) ligand [(11)C]carfentanil is a selective agonist for mu-opioid receptors and has been used for studying mu-opioid receptors in the human brain. However, it is unknown if [(11)C]carfentanil binding differentiates between subtype receptors mu1 and mu2. In this study, we investigated whether mu1 and mu2 can be studied separately through receptor subtype-selective inhibition of [(11)C]carfentanil by pharmacologic intervention. [(11)C]Carfentanil binding characteristics on rat brain sections were assessed either alone or in the presence of the mu-receptor inhibitor **cyprodime** or the mu1-specific inhibitor **naloxonazine**. [(11)C]Carfentanil binding in the living rat brain was similarly studied by small animal PET/computed tomography during baseline conditions or following displacement by **cyprodime** or **naloxonazine**. Autoradiography binding studies on rat brain sections demonstrated that [(11)C]carfentanil has higher affinity and binding potential for mu1 than for mu2. [(11)C]Carfentanil binding to mu2 in vivo could not be detected following specific blocking of mu1, as predicted from the low binding potential for mu2 as measured in vitro. [(11)C]Carfentanil binding is preferential for mu1 compared to mu2 in vitro and in vivo. Clinical studies employing [(11)C]carfentanil are therefore likely biased to measure mu1 rather than mu2.

***PMID:26461068***

*Eriksson O, Antoni G; Mol Imaging 14:476-83 (2015)*

**Hazardous Substances Data Bank (HSDB)**

# 9 Use and Manufacturing

## 9.1 Uses

**EPA CPDat Chemical and Product Categories**

*The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products, Scientific Data, volume 5, Article number: 180125 (2018),* ***DOI:10.1038/sdata.2018.125***

▸ **EPA Chemical and Products Database (CPDat)**

(11)C-Carfentanil has been widely used in positron emission tomography (PET) studies for measuring micro-opioid receptor binding in humans . ...

***PMID:18779961***
*Hirvonen J et al; Eur J Nucl Med Mol Imaging 36 (2): 275-86 (2009)*

▸ **Hazardous Substances Data Bank (HSDB)**

MEDICATION (VET)

▸ **Hazardous Substances Data Bank (HSDB)**

Carfentanil (DEA Code Number: 9743) is a Schedule II controlled substance.

*21 CFR 1308.12(c)(6) (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of April 25, 2017:* ***https://www.ecfr.gov***

▸ **Hazardous Substances Data Bank (HSDB)**

Schedule II Controlled Substance: (A) The drug or other substance has a high potential for abuse; (B) The drug or other substance has a currently accepted medical use in treatment in the United States or a currently accepted medical use with severe restrictions; and (C) Abuse of the drug or other substances may lead to severe psychological or physical dependence.

*US Department of Justice/Office of Diversion Control; Schedule of Controlled Substances. Available from, as of April 25, 2017:* ***https://www.deadiversion.usdoj.gov/21cfr/21usc/812.htm***

▸ **Hazardous Substances Data Bank (HSDB)**

For more Uses (Complete) data for Carfentanil (6 total), please visit the **HSDB record page**.

▸ **Hazardous Substances Data Bank (HSDB)**

## 9.2 Formulations/Preparations

The product is supplied as a sterile solution for parenteral administration into a large muscle mass at a dosage ranging from 0.005 to 0.020 milligrams per kilogram of body weight, Wildnil. /Carfentanil citrate/

*US FDA; Freedom of Information Act (FOIA) Drug Summaries. Wildnil. NADA 139-633. Available from, as of May 11, 2017:* ***https://www.fda.gov/downloads/AnimalVeterinary/Products/ApprovedAnimalDrugProducts/FOIADrugSummaries/UCM473748.pdf***

- **Hazardous Substances Data Bank (HSDB)**

## 9.3 General Manufacturing Information

Carfentanil is about 10,000 times as potent as morphine.

*Sams R; Vetinerary Drugs. Ullmann's Encyclopedia of Industrial Chemistry 7th ed. (1999-2017). NY, NY: John Wiley & Sons. Online Posting Date: June 15, 2000*

- **Hazardous Substances Data Bank (HSDB)**

# 10 Identification

## 10.1 Analytic Laboratory Methods

**Fentanyl** and **fentanyl** analogues represent a current and emerging threat in the United States as pure illicit narcotics and in mixtures with **heroin**. Because of their extreme potency, methods to safely and rapidly detect these compounds are of high interest. This work investigates the use of thermal desorption direct analysis in real time mass spectrometry (TD-DART-MS) and ion mobility spectrometry (IMS) as tools for the rapid and sensitive (nanogram to picograms) detection of **fentanyl**, 16 **fentanyl** analogues /including carfentanil/, and five additional opioids. Competitive ionization studies highlight that detection of these compounds in the presence of **heroin** is readily achievable, down to 0.1% **fentanyl** by mass with TD-DART-MS. With IMS, detection of nanogram levels of **fentanyl** in a binary **fentanyl** and **heroin** mixture is possible but can be complicated by decreased resolution in certain commercial instrument models. Modifications to the alarm windows can be used to ensure detection of **fentanyl** in binary mixtures. Additionally, three complex background matrices (fingerprint residue, dirt, and plasticizers) are shown to have a minimal effect of the detection of these compounds. Wipe sampling of the exterior of bags of questioned powders is shown to be a safe alternative method for field screening and identification, removing the need to handle potentially **lethal** amounts of material.

*Sisco E et al; Forensic Chemistry 4: 108-15 (2017)*

▸ **Hazardous Substances Data Bank (HSDB)**

## 10.2 Clinical Laboratory Methods

A sensitive, semiautomated method for the analysis of several fentanils /including **sufentanil** and carfentanil/ and **fentanil** metabolites in human urine is described. This method uses solid-phase extraction of urine samples followed by liquid chromatography-atmospheric pressure ionization-tandem mass spectrometry. Isotopically labeled internal standards were included for 6 of the 13 analytes in this study. Estimated detection limits ranged from 3 to 27 pg/mL, and good accuracy and long-term precision were observed in most cases. This method should be useful for the rapid and sensitive screening of human urine samples for a number of fentanils and their metabolites as indicators of exposure.

***PMID:16839472***
*Wang L, Bernert JT; J Anal Toxicol 30 (5): 335-41 (2006)*

▸ **Hazardous Substances Data Bank (HSDB)**

We have developed and evaluated a one step enzyme-linked immunosorbent assay (ELISA) test for **sufentanil** and a 125I radioimmunoassay test for **alfentanil** as part of a panel of pre- and post-race tests for narcotic analgesics in racing horses. Our **sufentanil** ELISA test detects **sufentanil** with an I-50 of about 0.5 ng/mL. The test is rapid and economical in that it can be read with an inexpensive spectrophotometer, or even by eye. The test readily detects the presence of **sufentanil** or its metabolites in equine blood and urine from 1 to 24 hours respectively after administration of therapeutic or sub-therapeutic doses of this drug. Our **sufentanil** assay also cross-reacts with **fentanyl**, the methylated analogs of **fentanyl** (designer fentanyls), and carfentanil and detected these drugs in urine for several hours after their administration to horses. It does not, however, cross-react significantly with **alfentanil**. We have also developed an 125I radioimmunoassay for **alfentanil**. This test allows detection of **alfentanil** in blood and urine of horses for up to 4 hours after administration of this drug. As such, these tests are capable of improving the quality and reducing the cost of pre-race and post-race testing for **fentanyl**, **sufentanil**, carfentanil and **alfentanil** and a number of their congeners in racing horses. Similarly, these tests are capable of screening for these drugs in human drug abuse monitoring.

***PMID:2521746***
*Tobin T et al; Res Commun Chem Pathol Pharmacol 63 (1): 129-52 (1989)*

▸ **Hazardous Substances Data Bank (HSDB)**

# 11 Safety and Hazards

## 11.1 Accidental Release Measures

### 11.1.1 Disposal Methods

SRP: Expired or waste pharmaceuticals shall carefully take into consideration applicable DEA, EPA, and FDA regulations. It is not appropriate to dispose by flushing the pharmaceutical down the toilet or discarding to trash. If possible return the pharmaceutical to the manufacturer for proper disposal being careful to properly label and securely package the material. Alternatively, the waste pharmaceutical shall be labeled, securely packaged and transported by a state licensed medical waste contractor to dispose by burial in a licensed hazardous or toxic waste landfill or incinerator.

- Hazardous Substances Data Bank (HSDB)

### 11.1.2 Preventive Measures

Carfentanil and other **fentanyl**-related compounds are a serious danger to public safety, first responder, medical, treatment, and laboratory personnel. ... If encountered, responding personnel should do the following based on the specific situation: Exercise extreme caution. Only properly trained and outfitted law enforcement professionals should handle any substance suspected to contain **fentanyl** or a **fentanyl**-related compound. If encountered, contact the appropriate officials within your agency. Be aware of any sign of exposure. Symptoms include: respiratory depression or arrest, drowsiness, disorientation, sedation, pinpoint pupils, and clammy skin. The onset of these symptoms usually occurs within minutes of exposure. Seek IMMEDIATE medical attention. Carfentanil and other **fentanyl**-related substances can work very quickly, so in cases of suspected exposure, it is important to call EMS immediately. ...

*DEA; DEA Issues Carfentanil Warning to Police and Public (September 22, 2016). Available from, as of June 30, 2017:* ***https://www.dea.gov/divisions/hq/2016/hq092216.shtml***

- Hazardous Substances Data Bank (HSDB)

## 11.2 Regulatory Information

### 11.2.1 FDA Requirements

Implantation or injectable dosage form new animal drugs. Carfentanil. ... Indications for use. For immobilizing free ranging and confined members of the family Cervidae (deer, elk, and moose). ... Limitations. Do not use in domestic animals intended for food. Do not use 30 days before or during hunting season. Federal law restricts this drug to use by or on the order of a licensed veterinarian. The licensed veterinarian shall be a veterinarian engaged in zoo and exotic animal practice, wildlife management programs, or research.

*21 CFR 522.300 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of April 25, 2017:* ***https://www.ecfr.gov***

- Hazardous Substances Data Bank (HSDB)

The Generic Animal Drug and Patent Restoration act requires that each sponsor of an approved animal drug must submit to the FDA certain information regarding patents held for the animal drug or its method of use. The Act requires that this information, as well as a list of all animal drug products approved for safety and effectiveness, be made available to the public. **Carfentanil citrate** is included on this list. /**Carfentanil citrate**/

*US FDA/Center for Veterinary Medicine; The Green Book - On Line, Active Ingredients. Carfentanil Citrate (61380-27-6). Available from, as of April 25, 2017:* ***https://www.fda.gov/AnimalVeterinary/Products/ApprovedAnimalDrugProducts/default.htm***

- Hazardous Substances Data Bank (HSDB)

Schedule II shall consist of the drugs and other substances, by whatever official name, common or usual name, chemical name, or brand name designated, listed in this section. Each drug or substance has been assigned the DEA Controlled Substances Code Number set forth opposite it. ... Opiates. Unless specifically excepted or unless in another schedule any of the following opiates, including its isomers, esters, ethers, salts and salts of isomers, esters and ethers whenever the existence of such isomers, esters, ethers, and salts is possible within the specific chemical designation, **dextrorphan** and **levopropoxyphene** excepted:. Carfentanil (DEA Code Number: 9743) is included on this list.

*21 CFR 1308.12(c)(6) (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of April 25, 2017: **https://www.ecfr.gov***

▶ Hazardous Substances Data Bank (HSDB)

## 11.3 Other Safety Information

### 11.3.1 History and Incidents

On October 26, 2002, Russian Special Forces deployed a chemical aerosol against Chechen terrorists to rescue hostages in the Dubrovka theatre. Its use confirmed Russian military interest in chemicals with effects on personnel and caused 125 deaths through a combination of the aerosol and inadequate medical care. This study provides evidence from liquid chromatography-tandem mass spectrometry analysis of extracts of clothing from two British survivors, and urine from a third survivor, that the aerosol comprised a mixture of two anaesthetics--carfentanil and **remifentanil**--whose relative proportions this study was unable to identify. Carfentanil and **remifentanil** were found on a shirt sample and a metabolite called **norcarfentanil** was found in a urine sample. This metabolite probably originated from carfentanil.

***PMID:23002178***
*Riches JR et al; J Anal Toxicol 36 (9): 647-56 (2012)*

▶ Hazardous Substances Data Bank (HSDB)

In October 2002, the Russian military used a mysterious "gas" to incapacitate Chechen rebels at a Moscow theater. Despite increased interest in the potential use of **lethal** chemical weapons in recent years, the medical community has paid little attention to the development of incapacitating, calmative, and "less than **lethal**" technologies. In this analysis, we review the events surrounding the use of a calmative "gas" during the Russian military action and discuss what is currently known about **fentanyl** derivatives, their aerosolization, and the rationale for their use as incapacitating agents. Collectively, the available evidence strongly suggests that a combination of a potent aerosolized **fentanyl** derivative, such as carfentanil, and an inhalational anesthetic, such as **halothane**, was used. The paper also assesses potential errors leading to the loss of a substantial number of hostages. Several lessons can be learned from this surprising and novel use of an incapacitating gas.

***PMID:12712038***
*Wax PM et al; Ann Emerg Med 41 (5): 700-5 (2003)*

▶ Hazardous Substances Data Bank (HSDB)

### 11.3.2 Special Reports

Vardanyan RS, Hruby; **Fentanyl**-related Compounds and Derivatives: Current Status and Future Prospects for Pharmaceutical Applications; Future Med Chem 6 (4): 385-412 (2014)

▶ Hazardous Substances Data Bank (HSDB)

# 12 Toxicity

## 12.1 Toxicological Information

### 12.1.1 Toxicity Summary

IDENTIFICATION AND USE: Carfentanil is a Schedule II controlled substance. It is a large animal immobilizing agent use in Cervidae (deer, elk, moose), and veterinary anesthetic used for zoo animals. Carfentanil is an ultra-potent synthetic opioid. These substances can come in several forms, including powder, blotter paper, tablets, and spray - they can be absorbed through the skin or accidental inhalation of airborne powder. HUMAN STUDIES: Carfentanil has been discovered in postmortem and antemortem cases throughout the United States in the **heroin** supply either alone or mixed with **heroin** and/or other **fentanyl** analogs. The potency of carfentanil is approximately 10,000 times greater than **morphine** and 100 times greater than **fentanyl**. In some cases, carfentanil was identified and ruled to be the cause of death, either alone or in combination with other drugs. In October 2002, the Russian military used a mysterious "gas" to incapacitate Chechen rebels at a Moscow theater. The available evidence strongly suggests that a combination of a potent aerosolized **fentanyl** derivative, such as carfentanil, and an inhalational anesthetic, such as **halothane**, was used in this case. Other study suggested that aerosol comprised a mixture of two anaesthetics -carfentanil and **remifentanil**. ANIMAL STUDIES: After **carfentanil citrate** administration, 3 horses developed severe tachycardia and hypertension, which resulted in the death of 1 horse from pulmonary edema. Intramuscularly administered **etorphine** and carfentanil induce hypertension, bradycardia, and bradypnea in goats. The mean dose of carfentanil used in wood bison was 7.0 ug/kg. Narcotic antagonists used were **naltrexone**, **naloxone** and M5050.

- Hazardous Substances Data Bank (HSDB)

### 12.1.2 Acute Effects

- ChemIDplus

### 12.1.3 Interactions

Using a crossover study design, the pharmacokinetics of carfentanil and **naltrexone** after i.v., i.m., and s.c. administration were determined in eight domestic goats (Capra hircus). Serial blood samples were taken up to 120 hr after carfentanil administration, and the plasma drug concentrations were determined using liquid chromatography and mass spectroscopy. All goats were immobilized with 40 ug/kg carfentanil i.m., although the resulting neurologic effects varied considerably. Plasma profiles showed rapid carfentanil absorption and a simple biphasic decline for 12-48 hr. **Naltrexone** given at 100 mg **naltrexone**/mg carfentanil

30 min after carfentanil administration produced rapid reversal of immobilization after all routes of administration. Variable fluctuations in the **naltrexone** plasma concentrations during the first 2.5-3.5 hr were observed, followed by a more consistent biphasic decline. The time to standing was significantly shorter after i.v. compared with s.c. **naltrexone**, although the time difference (1 min) had little clinical relevance. No statistically significant differences between the **naltrexone** pharmacokinetic parameters measured for the three routes of **naltrexone** administration were identified, although the recoveries after i.m. administration were, subjectively, the smoothest. The carfentanil half-life did not differ significantly in the goats given **naltrexone** by different routes. Although it is currently recommended that the **naltrexone** dose be divided into s.c. and i.v. portions, this practice does not appear to offer any benefit.

***PMID:15732589***

*Mutlow A et al; J Zoo Wildl Med 35 (4): 489-96 (2004)*

▸ **Hazardous Substances Data Bank (HSDB)**

With the use of a crossover study design, we investigated the respiratory and cardiovascular effects of **naloxone** administration in eight healthy Rocky Mountain wapiti (Cervus elaphus nelsoni) anesthetized with carfentanil (10 ug/kg i.m.) and **xylazine** (0.1 mg/kg). Anesthetized animals showed profound hypoxemia with mild hypercapnia, tachycardia, hypertension, and acidosis prior to **naloxone** administration. After monitoring equipment was placed, animals were administered either **naloxone** (2 ug/ug carfentanil i.v.) or an equivalent volume of normal saline. Mean values for PaO2, PaCO2, heart rate, and respiratory rate were significantly different between **naloxone**- and saline-treated groups, but mean blood pressure, hematocrit, and serum electrolyte concentrations were not. Mean PaO2 was 23.0 +/- 4.1 mm Hg prior to administration of **naloxone** or saline and increased to 50.2 +/- 7.3 mm Hg after **naloxone** administration. Mean PaO2 of saline-treated animals did not change significantly. Electrocardiograms of three saline-treated animals suggested myocardial hypoxia. Hypoxemia appeared to be caused by respiratory depression, hemodynamic alterations, and lateral recumbency. All but one animal remained anesthetized after **naloxone** administration. Anesthesia in all animals was reversed in < or = 4 min with naltrexone (100 mg/mg carfentanil i.v. s.c.) and yohimbine (0.1 mg/kg i.v.). One bolus of naloxone improved oxygenation in carfentanil-xylazine-anesthetized wapiti.

***PMID:12790400***

*Moresco A et al; J Zoo Wildl Med 32 (1): 81-9 (2001)*

▸ **Hazardous Substances Data Bank (HSDB)**

Reversing the respiratory depression induced by carfentanil involves intravenous administration of **naloxone** or **naltrexone**, but this treatment has disadvantages. Hence, finding a more appropriate treatment to counter the depressive actions of carfentanil is needed. In the present study, with the **naloxone** as a control, we investigated the efficacy of **nalmefene** for countering the depressive actions of carfentanil. Rats were treated successively with carfentanil (10 ug/kg, i.v.) and **nalmefene** (9.4-150.0 ug/kg, i.m.), and the duration of loss of righting reflex (LORR) recorded. Respiratory parameters were measured in free-moving rats using a whole-body plethysmograph after rats were administered carfentanil (20 ug/kg, i.v.) and **nalmefene** (9.4-150.0 ug/kg, i.m.) sequentially. The parameters of arterial blood gases were also examined. **Nalmefene** (9.4-150.0 ug/kg, i.m.) treatment dose-dependently decreased the duration of carfentanil-induced LORR. The respiratory rate after 60 min of **nalmefene** (150.0 ug/kg, i.m.) treatment increased from 34.3 +/- 5.3 bursts/min to 117.8 +/- 18.9 bursts/min, and enhanced pause decreased from 1.1 +/- 0.1 to 0.4 +/- 0.1, and was close to those of normal rats. Furthermore, **nalmefene** (37.5-150.0 ug/kg) treatment could enable the PaO2, SaO2 and PaCO2 to approach normal levels 10 min (15 min after carfentanil injection) or 30 min (25 min after carfentanil injection) after injection. While, a single injection of **naloxone** (150.0 ug/kg, i.m.) only achieved partial remission of respiratory depression. These data suggest that **nalmefene** more effectively counters the depressive actions induced by carfentanil and is a more appropriate treatment to antagonize carfentanil toxicity compared with **naloxone**.

***PMID:24886878***

*Yong Z et al; Eur J Pharmacol. 2014 Sep 5;738:153-7 (2014)*

▸ **Hazardous Substances Data Bank (HSDB)**

We evaluated efficacy and safety of **naltrexone** for antagonizing carfentanil immobilization in 12 captive Rocky Mountain elk (Cervus elaphus nelsoni) using a randomized incomplete block experiment. In three replicate trials, elk were hand-injected with 10 micrograms **carfentanil citrate**/kg body weight intramuscularly. Fifteen min after each elk became recumbent, we administered **naltrexone HCl** (25% of dose intravenously, 75% subcutaneously) dosed at 0 (control), 25, 50, or 100 mg/mg carfentanil; after an additional 15 min of immobilization, controls received 500 mg **naltrexone HCl**/mg carfentanil. Elk were immobilized in 34 of 36 attempts; the mean (+/-SE) induction time was 3.1 +/- 0.2 min. Regardless of dose, all elk stood < 9 min

after receiving naltrexone; controls remained immobilized until they received antagonist. Mean recovery times did not differ with increasing naltrexone dose (P = 0.31) or among individuals (P = 0.16). None of the elk receiving 100 or 500 mg naltrexone/mg carfentanil renarcotized, but three of eight and seven of nine elk receiving 50 and 25 mg naltrexone/mg carfentanil, respectively, showed signs of mild renarcotization 8 to 24 hr later (P = 0.0002). We observed no adverse clinical effects in elk receiving < or = 500 mg naltrexone/mg carfentanil. Based on these data, we recommend 100 mg/mg carfentanil as a minimum effective dose for rapidly antagonizing immobilization and preventing renarcotization.

*PMID:8722260*

*Miller MW et al; J Wildl Dis 32 (2): 234-9 (1996)*

Hazardous Substances Data Bank (HSDB)

For more Interactions (Complete) data for Carfentanil (8 total), please visit the **HSDB record page**.

Hazardous Substances Data Bank (HSDB)

## 12.1.4 Antidote and Emergency Treatment

/SRP:/ Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing **water**. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Poisons A and B/

*Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160*

Hazardous Substances Data Bank (HSDB)

/SRP:/ Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if needed. Administer **oxygen** by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary ... . Monitor for shock and treat if necessary ... . Anticipate seizures and treat if necessary ... . For eye contamination, flush eyes immediately with **water**. Irrigate each eye continuously with 0.9% saline (NS) during transport ... . Do not use emetics. For ingestion, rinse mouth and administer 5 mL/kg up to 200 mL of **water** for dilution if the patient can swallow, has a strong gag reflex, and does not drool ... . /Poisons A and B/

*Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160*

Hazardous Substances Data Bank (HSDB)

/SRP:/ Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Positive-pressure ventilation techniques with a bag valve mask device may be beneficial. Consider drug therapy for pulmonary edema ... . Consider administering a beta agonist such as **albuterol** for severe bronchospasm ... . Monitor cardiac rhythm and treat arrhythmias as necessary ... . Start IV administration of D5W TKO /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's (LR) if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Watch for signs of fluid overload ... . Treat seizures with **diazepam** or **lorazepam** ... . Use **proparacaine hydrochloride** to assist eye irrigation ... . /Poisons A and B/

*Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160-1*

Hazardous Substances Data Bank (HSDB)

Emergency and supportive measures. 1. Maintain an open airway and assist ventilation if necessary. Administer supplemental **oxygen**. Treat coma, seizures, hypotension, and noncardiogenic pulmonary edema if they occur. /Opiates and opioids/

*OLSON, K.R. (Ed). Poisoning and Drug Overdose, Sixth Edition. McGraw-Hill, New York, NY 2012, p. 312*

Hazardous Substances Data Bank (HSDB)

For more Antidote and Emergency Treatment (Complete) data for Carfentanil (9 total), please visit the **HSDB record page**.

▶ **Hazardous Substances Data Bank (HSDB)**

## 12.1.5 Human Toxicity Excerpts

/CASE REPORTS/ Recreational use of potent **fentanyl** derivatives is increasing and poses a serious threat to health and public safety. The **fentanyl** derivative carfentanil, a large animal tranquilizer, is one of the most potent opioids known (10,000 times more potent than **morphine**) and can lead to severe or fatal intoxications even among opioid-tolerant users. **Naloxone** can be lifesaving in acute intoxications. The substance should be handled with utmost caution, as even inhalation, dermal or mucosal exposure can lead to intoxication. We report a case of confirmed acute carfentanil intoxication in Switzerland in order to contribute to the scarce knowledge of its toxicodynamic properties in humans. Case report: A 16-year-old male was admitted to the intensive care unit after sudden collapse, reportedly following the intake of an unknown drug via an unknown route. His regular medications were **atomoxetine** and **mirtazapine**. The patient was found unconscious (Glasgow Coma Scale 3/15), hypotensive (71/58 mmHg), tachycardic (126 beats per minute), apneic and cyanotic with peripheral **oxygen** saturation of 70%. Temperature and pupil findings were normal. After intubation, he was airlifted to the emergency department, where, after intravenous **naloxone** and **flumazenil**, he rapidly regained consciousness, becoming agitated and hypertensive. Other investigations including focused sonography, electrocardiogram, head computed tomography and laboratory analyses were normal except for mild respiratory acidosis. Urine drug screening immunoassay was negative twice. When a white powder along with a snorting tube were found in the patient's belongings, **cocaine** intoxication was suspected, but gas chromatography-mass spectrometry (GC-MS) and liquid chromatography combined with high resolution tandem mass spectrometry (LC-MS/MS) both identified the powder as carfentanil. Traces of carfentanil were also detected in blood using LC-MS/ MS. According to the caretaking institution, the patient was known for online substance acquisitions for self-experimenting and trafficking. He was discharged the day after the event. Conclusion: Recreational use of carfentanil caused sudden deep coma, hypotension and respiratory arrest responsive to **naloxone**.

*Muller S et al; Clin Toxicol (Phila) 55 (5): 371-544 (2017)*

▶ **Hazardous Substances Data Bank (HSDB)**

/CASE REPORTS/ Carfentanil is a **fentanyl** analog frequently used in large animal veterinary medicine. Recently, carfentanil has been discovered in postmortem and antemortem cases throughout the United States in the **heroin** supply either alone or mixed with **heroin** and/or other **fentanyl** analogs. The potency of carfentanil is approximately 10,000 times greater than **morphine** and 100 times greater than **fentanyl**. In two recent cases, carfentanil was identified and ruled to be the cause of death, either alone or in combination with other drugs. Case 1 involved a known **heroin** user. He was discovered slumped over in a running van blocking the bays of a carwash. Two syringes, a spoon with cotton and residue and a yellow baggie of powder were found in the van. Case 2 involved a man living in a tent in a park with his mother. He was last heard from by a sister via phone who stated he sounded very intoxicated and by his mother who noted him to be "itching all over" and upset over his girlfriend. When the mother returned from work, she discovered him unresponsive with a small baggie of brown powder next to him. Routine drug and volatile screening tests were performed on heart blood using headspace gas chromatography, immunoassay and gas chromatography mass spectrometry methods. Results from initial testing on both cases did not have any significant toxicological findings. However, due to the history, scene photos, toxicological findings in blood and urine and analysis of the drug paraphernalia on one of the cases which identified carfentanil and furanyl **fentanyl**, **fentanyl** analogues were suspected. Heart blood was sent to a reference laboratory for carfentanil and furanyl **fentanyl** analysis. Case 1 had a carfentanil concentration of 1.3 ng/mL and a furanyl **fentanyl** concentration of 0.34 ng/mL. Case 2 had a carfentanil concentration of 0.12 ng/mL.

***PMID:28575422***
*Swanson DM et al; J Anal Toxicol 31:1-5 (2017)*

▶ **Hazardous Substances Data Bank (HSDB)**

/OTHER TOXICITY INFORMATION/ DEA has issued a public warning to the public and law enforcement nationwide about the health and safety risks of carfentanil. Carfentanil is a synthetic opioid that is 10,000 times more potent than **morphine** and 100 times more potent than **fentanyl**, which itself is 50 times more potent than **heroin**. DEA, local law enforcement and first responders have recently seen the presence of carfentanil, which has been linked to a significant number of overdose deaths in various parts of the country. Improper handling of carfentanil, as well as **fentanyl** and other **fentanyl**-related compounds, has

deadly consequences. ... Carfentanil is a Schedule II substance under the Controlled Substances Act and is used as a tranquilizing agent for elephants and other large mammals. The **lethal** dose range for carfentanil in humans is unknown. However, as noted, carfentanil is approximately 100 times more potent than **fentanyl**, which can be **lethal** at the 2-milligram range, depending on route of administration and other factors. Carfentanil and other **fentanyl**-related compounds are a serious danger to public safety, first responder, medical, treatment, and laboratory personnel. These substances can come in several forms, including powder, blotter paper, tablets, and spray - they can be absorbed through the skin or accidental inhalation of airborne powder.

*DEA; DEA Issues Carfentanil Warning to Police and Public (September 22, 2016). Available from, as of June 30, 2017:* ***https://www.dea.gov/divisions/hq/2016/hq092216.shtml***

▶ **Hazardous Substances Data Bank (HSDB)**

/OTHER TOXICITY INFORMATION/ In October 2002, the Russian military used a mysterious "gas" to incapacitate Chechen rebels at a Moscow theater. Despite increased interest in the potential use of **lethal** chemical weapons in recent years, the medical community has paid little attention to the development of incapacitating, calmative, and "less than **lethal**" technologies. In this analysis, we review the events surrounding the use of a calmative "gas" during the Russian military action and discuss what is currently known about **fentanyl** derivatives, their aerosolization, and the rationale for their use as incapacitating agents. Collectively, the available evidence strongly suggests that a combination of a potent aerosolized **fentanyl** derivative, such as carfentanil, and an inhalational anesthetic, such as **halothane**, was used. The paper also assesses potential errors leading to the loss of a substantial number of hostages. Several lessons can be learned from this surprising and novel use of an incapacitating gas.

***PMID:12712038***
*Wax PM et al; Ann Emerg Med 41 (5): 700-5 (2003)*

▶ **Hazardous Substances Data Bank (HSDB)**

For more Human Toxicity Excerpts (Complete) data for Carfentanil (6 total), please visit the **HSDB record page**.

▶ **Hazardous Substances Data Bank (HSDB)**

## 12.1.6 Non-Human Toxicity Excerpts

/LABORATORY ANIMALS: Acute Exposure/ This study examined the real-time exposure-response effects of aerosolized carfentanil (CRF) on opioid-induced toxicity, respiratory dynamics and cardiac function in mice. Unrestrained, conscious male CD-1 mice (25-30 g) were exposed to 0.4 or 4.0 mg/cu m of aerosolized CRF for 15 min (Ct = 6 or 60 mg min/cu m) in a whole-body plethysmograph chamber. Minute volume (MV), core body temperature (Tc), mean arterial blood pressure (MAP) and heart rate (HR) were evaluated in animals exposed to CRF or sterile H2O. Loss of consciousness and Straub tail were observed in before 1 min following initiation of exposure to 6 or 60 mg min/cu m of CRF. Clinical signs of opioid-induced toxicity were observed in a dose-dependent manner. Exposure to 6 or 60 mg min/cu m of CRF resulted in significant decrease in MV as compared to the controls. MAP, HR and Tc decreased 24 hr in animals exposed to either 6 or 60 mg min/cu m of CRF as compared to the controls. Post-exposure administration of **naloxone** (NX, 0.05 mg/kg, i.m.) did not increase the MV of animals exposed to CRF to control levels within 24 hr, but decreased clinical signs of opioid-induced toxicity and the duration of respiratory depression. This is the first study to evaluate real-time respiratory dynamics and cardiac function during exposure and up to 24 hr post-exposure to CRF. The evaluation of toxicological signs and respiratory dynamics following exposure to CRF will be useful in the development of therapeutic strategies to counteract the ongoing threat of abuse and overuse of opioids and their synthetic variants.

***PMID:28330429***
*Wong B et al; Inhal Toxicol 29 (2): 65-74 (2017)*

▶ **Hazardous Substances Data Bank (HSDB)**

/VETERINARY CASE REPORTS/ Ten black bears (Ursus americanus) were immobilized with orally administered **carfentanil citrate**. The total carfentanil dose was mixed with 5 to 20 mL honey and given incrementally to captive bears. The bears ranged in weight from 80 (estimated) to 233 kg. Total carfentanil doses ranged from 0.7 to 3.0 mg, resulting in dosages of 6.8 to 18.8 ug carfentanil/kg. Mean (+/- SD) times from estimated 80% mixture consumption to sternal recumbency, and first safe human contact were 7.7 +/- 2.3 min and 19.7 +/- 5.6 min, respectively. Undesired side effects of immobilization were muscle rigidity,

bradypnea, and **oxygen** desaturation. All bears received **diazepam** to alleviate muscle rigidity and were insufflated with **oxygen** during immobilization. Nine immobilizations were considered satisfactory or good. The bear receiving 6.8 ug carfentanil/kg, the lowest dosage used, was very excited during induction and required intravenous (IV) **ketamine** to permit safe examination. Immobilization was reversed with 100 mg **naltrexone**/mg carfentanil administered (75% subcutaneous, 25% IV). Bears recovered to full mobility in 6.3 +/- 1.9 min. Five bears vomited post-recovery but no episodes of renarcotization were observed.

***PMID:8592362***

*Ramsay EC et al; J Wildl Dis 31 (3): 391-3 (1995)*

**Hazardous Substances Data Bank (HSDB)**

/VETERINARY CASE REPORTS/ /The purpose of this study was/ to determine comparative cardiopulmonary effects of IM administered **etorphine** and carfentanil in goats. Seven clinically normal adult female goats ... received at least 9 drug treatments (**etorphine HCl**, 5 [twice], 10, 20, and 40 and **carfentanil citrate**, 5, 10, 20 and 40 ug/kg of body weight), with a minimal 2-day interval between trials. Although drug dosages were randomized, **etorphine** and carfentanil treatments were alternated. To assess for drug tolerance, the first and last treatments always were **etorphine** (5 ug/kg). All goats were instrumented for long-term cardiopulmonary variable data collection. Both drugs induced rapid catatonic immobilization, characterized by limb and neck hyperextension, with occasional vocalization and bruxation. **Etorphine** elicited transient violent struggling and vocalization immediately. Time to immobilization appeared dose-dependent, and was more rapid with carfentanil (< or = 5 minutes) than etorphine (5 to 10 minutes) at all dosages. Recovery to standing occurred earlier for etorphine (1 to 2 hours) than carfentanil (> 2 hours) at all dosages. Both drugs at all dosages significantly (P < or = 0.05) increased systemic and left ventricular (LV) end-diastolic pressures, LV peak negative dP/dt, total peripheral resistance (TPR), hemoglobin concentration, and left atrial (LA) and pulmonary O2 contents. They also significantly decreased heart and respiration rates, and TPR. A significant increase was observed at some dosages for LV stroke volume and index, LV peak positive dP/dt, mean pulmonary artery pressure, PaO2, pulmonary artery oxygen partial pressure, PaCO2, pulmonary mixed venous carbon dioxide partial pressure, LA hemoglobin saturation, LA transport index, and body temperature. Pulmonary and systemic mixed venous carbon dioxide and oxygen contents were significantly decreased at some dosages. Intramuscularly administered etorphine and carfentanil induce hypertension, bradycardia, and bradypnea in goats. The hypertension appears attributable to an increase in TPR. Although the cardiopulmonary effects of carfentanil occurred more rapidly, these effects were similar in magnitude for etorphine and carfentanil over the evaluated dosage range.

***PMID:8720245***

*Heard DJ et al; Am J Vet Res 57 (1): 87-96 (1996)*

**Hazardous Substances Data Bank (HSDB)**

/VETERINARY CASE REPORTS/ /The purpose of this study was/ to determine the effects of an i.m. administered carfentanil-**xylazine** combination on cardiopulmonary variables and plasma **catecholamine** concentrations and to validate use of pulse oximetry in bongo antelopes. Eight healthy adult female antelopes were immobilized with **carfentanil citrate** (8.3 ug/kg of body weight, i.m.) and **xylazine hydrochloride** (0.79 mg/kg, i.m.). Hematologic values and plasma biochemical and **catecholamine** concentrations were determined at the beginning and end of immobilization. Immediately after induction of immobilization and every 15 minutes thereafter, cardiopulmonary variables were determined. Induction time after carfentanil-**xylazine** administration was 6 +/- 2 minutes. At 15 and 45 minutes after immobilization and thereafter, significant decrease in heart and respiratory rates, respectively, were observed. After 15 minutes of immobilization, all antelopes had developed mild hypoxemia, which resolved after nasal insufflation with 100% **oxygen**. Pulse oximetry readings underestimated arterial blood gas values, but reliably indicated trends in arterial **oxygen** desaturation. Antelopes developed hypoxemia after **oxygen** administration was terminated at the end of the procedure, prior to reversal of immobilization. **Norepinephrine** concentrations increased significantly (P < 0.05), and 3,4-dihydroxyphenylacetic acid concentrations decreased significantly at the end of the anesthetic event. Immobilization of all antelopes was reversed, using antagonists naltrexone and yohimbine hydrochloride. Time to standing was 3 +/- 1 minutes, and renarcotization was not observed. The carfentamil-xylazine combination at the dosage used induced hypoxemia, pronounced arterial hypertension, and significant increase in plasma norepinephrine and decrease in plasma 3,4-dihydroxyphenylacetic acid concentrations in bongo antelopes. Supplemental administration of oxygen is recommended. Pulse oximetry is a useful tool to monitor trends in arterial oxygen desaturation, but does not substitute for arterial blood gas analysis.

***PMID:9028481***

*Schumacher J et al; Am J Vet Res 58 (2): 157-61 (1997)*

Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Excerpts (Complete) data for Carfentanil (7 total), please visit the **HSDB record page**.

Hazardous Substances Data Bank (HSDB)

## 12.2 Ecological Information

### 12.2.1 Environmental Fate/Exposure Summary

Carfentanil's production and use as a radiotracer in positron emission tomography(PET) and a large animal tranquilizer may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 2X10-10 mm Hg at 25 °C indicates carfentanil will exist solely in the particulate phase in the atmosphere. Particulate-phase carfentanil will be removed from the atmosphere by wet and dry deposition. Carfentanil contains chromophores that absorb at wavelengths >290 nm and, therefore, may be susceptible to direct photolysis by sunlight. If released to soil, carfentanil is expected to have no mobility based upon an estimated Koc of 18,000. The estimated pKa of carfentanil is 8.05, indicating that this compound will exist partially in the cation form in the environment and cations generally adsorb more strongly to soils containing organic **carbon** and clay than their neutral counterparts. Volatilization from moist soil surfaces is not expected to be an important fate process based upon the estimated pKa and an estimated Henry's Law constant of 4.4X10-13 atm-cu m/mole. Carfentanil is not expected to volatilize from dry soil surfaces based upon its estimated vapor pressure. Biodegradation data in soil or **water** were not available. If released into **water**, carfentanil is expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from **water** surfaces is not expected to be an important fate process based upon this compound's estimated pKa and Henry's Law constant. An estimated BCF of 80 suggests the potential for bioconcentration in aquatic organisms is moderate. Estimated hydrolysis half-lives are 35 and 3.5 years at pH values of 7 and 8, respectively. Occupational exposure to carfentanil may occur through dermal contact with this compound at workplaces where carfentanil is produced or administered. Exposure to carfentanil among the general population may be limited to its use as a PET imaging compound and as an illicit drug. (SRC)

Hazardous Substances Data Bank (HSDB)

### 12.2.2 Artificial Pollution Sources

Carfentanil's production and use as a radiotracer in positron emission tomography (PET)(1) and a large animal tranquilizer(2) may result in its release to the environment through various waste streams(SRC). It is a Schedule II controlled substance(3).[(1) Pecina M, Zubieta JK; Mol Psychiatry 20: 416-23 (2015) (2) Daughton CG; Rev Environ Contam Toxicol 210: 59-110 (2011) (3) DEA; Title 21 Code Fed Reg. Part 1308 - Schedules of Controlled Substances. Schedules. Sec 1308.12 Schedule II.

*39 FR 22141, June 20, 1974]. Available from, as of Jun 12, 2017:* ***https://www.deadiversion.usdoj.gov/21cfr/cfr/1308/1308_12.htm***

Hazardous Substances Data Bank (HSDB)

### 12.2.3 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 18,000(SRC), determined from a structure estimation method(2), indicates that carfentanil is expected to be immobile in soil(SRC). The estimated pKa of carfentanil is 8.05(3), indicating that this compound will exist partially in the cation form in the environment and cations generally adsorb more strongly to soils containing organic **carbon** and clay than their neutral counterparts(4). Volatilization of the cation form from moist soil is not expected because cations do not volatilize(SRC). Volatilization of neutral carfentanil from moist soil surfaces is not expected(SRC) given an estimated Henry's Law constant of 4.4X10-13 atm-cu m/mole(SRC), using a fragment constant estimation method(2). Carfentanil is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 2X10-10 mm Hg at 25 °C(SRC), determined from a fragment constant method(2). Biodegradation data in soil were not available(SRC, 2017).

*(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of May 8, 2017: **https://www2.epa.gov/tsca-screening-tools** (3) Wishart DS et al; Nucleic Acids Res 34: D668-72 (2006). Available from, as of May 11, 2017: **https://www.drugbank.ca/** (4) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000)*

▶ **Hazardous Substances Data Bank (HSDB)**

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 18,000(SRC), determined from a structure estimation method(2), indicates that carfentanil is expected to adsorb to suspended solids and sediment(SRC). An estimated pKa of 8.05(3) indicates carfentanil will exist partially in the cation form at pH values of 5 to 9 and, therefore, volatilization of the cation from **water** surfaces is not expected to be an important fate process(SRC). Volatilization from **water** surfaces of neutral carfentanil is not expected(4) based upon an estimated Henry's Law constant of 4.4X10-13 atm-cu m/mole(SRC), developed using a fragment constant estimation method(2). The estimated hydrolysis half-life of carfentanil at pH values of 7 and 8 was calculated as 35 and 3.5 years, respectively(2). According to a classification scheme(5), an estimated BCF of 80(SRC), from an estimated log Kow of 3.39(2) and a regression-derived equation(2), suggests the potential for bioconcentration in aquatic organisms is moderate. Biodegradation data in **water** were not available(SRC, 2017).

*(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of May 8, 2017: **https://www2.epa.gov/tsca-screening-tools** (3) Wishart DS et al; Nucleic Acids Res 34: D668-72 (2006). Available from, as of May 11, 2017: **https://www.drugbank.ca/** (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5, 15-1 to 15-29 (1990) (5) Franke C et al; Chemosphere 29: 1501-14 (1994)*

▶ **Hazardous Substances Data Bank (HSDB)**

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), carfentanil, which has an estimated vapor pressure of 2X10-10 mm Hg at 25 °C(SRC), determined from a fragment constant method(2), is expected to exist solely in the particulate phase in the ambient atmosphere. Particulate-phase carfentanil may be removed from the air by wet and dry deposition(SRC). Carfentanil contains chromophores that absorb at wavelengths >290 nm(3) and, therefore, may be susceptible to direct photolysis by sunlight(SRC).

*(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of May 8, 2017: **https://www2.epa.gov/tsca-screening-tools** (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-12, 8-13 (1990)*

▶ **Hazardous Substances Data Bank (HSDB)**

## 12.2.4 Environmental Abiotic Degradation

A base-catalyzed second-order hydrolysis rate constant of 0.0062 L/mole-sec(SRC) was estimated for carfentanil using a structure estimation method(1); this corresponds to half-lives of 35 and 3.5 years at pH values of 7 and 8, respectively(1). Carfentanil contains chromophores that absorb at wavelengths >290 nm(2) and, therefore, may be susceptible to direct photolysis by sunlight(SRC).

*(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of May 8, 2017: **https://www2.epa.gov/tsca-screening-tools** (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-12, 8-13 (1990)*

▶ **Hazardous Substances Data Bank (HSDB)**

## 12.2.5 Environmental Bioconcentration

An estimated BCF of 80 was calculated in fish for carfentanil(SRC), using an estimated log Kow of 3.39(1) and a regression-derived equation(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is moderate.

*(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of May 8, 2017: **https://www2.epa.gov/tsca-screening-tools/** (2) Franke C et al; Chemosphere 29: 1501-14 (1994)*

▶ **Hazardous Substances Data Bank (HSDB)**

## 12.2.6 Soil Adsorption/Mobility

Using a structure estimation method based on molecular connectivity indices(1), the Koc of carfentanil can be estimated to be 18,000(SRC). According to a classification scheme(2), this estimated Koc value suggests that carfentanil is expected to be immobile in soil. The estimated pKa of carfentanil is 8.05(3), indicating that this compound will exist partially in the cation form in the environment and cations generally adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(4).

*(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of May 8, 2017: **https://www2.epa.gov/tsca-screening-tools** (2) Swann RL et al; Res Rev 85: 17-28 (1983) (3) Wishart DS et al; Nucleic Acids Res 34: D668-72 (2006). Available from, as of May 11, 2017: **https://www.drugbank.ca/** (4) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000)*

▸ **Hazardous Substances Data Bank (HSDB)**

## 12.2.7 Volatilization from Water/Soil

An estimated pKa of 8.05(1) indicates carfentanil will exist partially in the cation form at pH values of 5 to 9 and, therefore, volatilization of the cation from water and moist soil surfaces is not expected to be an important fate process(SRC). The Henry's Law constant for carfentanil is estimated as 4.4X10-13 atm-cu m/mole(SRC) using a fragment constant estimation method(2). This Henry's Law constant indicates that neutral carfentanil is expected to be essentially nonvolatile from water and moist soil surfaces(3). Carfentanil is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 2X10-10 mm Hg(SRC), determined from a fragment constant method(2).

*(1) Wishart DS et al; Nucleic Acids Res 34: D668-72 (2006). Available from, as of May 11, 2017: **https://www.drugbank.ca/** (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of May 8, 2017: **https://www2.epa.gov/tsca-screening-tools** (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990)*

▸ **Hazardous Substances Data Bank (HSDB)**

## 12.2.8 Probable Routes of Human Exposure

Occupational exposure to carfentanil may occur through dermal contact with this compound at workplaces where carfentanil is produced or administered. Exposure to carfentanil among the general population may be limited to its use as a positron emission tomography (PET) imaging compound and as an illicit drug. (SRC)

▸ **Hazardous Substances Data Bank (HSDB)**

# 13 Literature

## 13.1 NLM Curated PubMed Citations

- PubChem

## 13.2 Springer Nature References

- Springer Nature

## 13.3 Thieme References

Thieme Chemistry

## 13.4 Depositor Provided PubMed Citations

PubChem

## 13.5 Synthesis References

Louis P. Reiff, Paul B. Sollman, "Process of making carfentanil and related analgesics." U.S. Patent US5106983, issued January, 1981.

DrugBank

## 13.6 General References

Wax PM, Becker CE, Curry SC: Unexpected "gas" casualties in Moscow: a medical toxicology perspective. Ann Emerg Med. 2003 May;41(5):700-5. [PMID:12712038]

DrugBank

## 13.7 Chemical Co-Occurrences in Literature

PubChem

## 13.8 Chemical-Gene Co-Occurrences in Literature

PubChem

## 13.9 Chemical-Disease Co-Occurrences in Literature

- PubChem

# 14 Patents

## 14.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

## 14.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=YDSDEBIZUNNPOB-UHFFFAOYSA-N

PATENTSCOPE (WIPO)

# 15 Biomolecular Interactions and Pathways

## 15.1 Drug-Gene Interactions

- Drug Gene Interaction database (DGIdb)

## 15.2 Chemical-Gene Interactions

### 15.2.1 CTD Chemical-Gene Interactions

- Comparative Toxicogenomics Database (CTD)

## 15.3 DrugBank Interactions

DrugBank

## 15.4 Drug-Drug Interactions

DrugBank

## 15.5 Pathways

- PubChem

# 16 Biological Test Results

## 16.1 BioAssay Results

- PubChem

# 17 Classification

## 17.1 Ontologies

### 17.1.1 MeSH Tree

- Medical Subject Headings (MeSH)

### 17.1.2 ChEBI Ontology

- ChEBI

### 17.1.3 KEGG: Target-based Classification of Drugs

KEGG

### 17.1.4 KEGG: Drug Classes

KEGG

### 17.1.5 ChemIDplus

- ChemIDplus

### 17.1.6 Guide to PHARMACOLOGY Target Classification

- IUPHAR/BPS Guide to PHARMACOLOGY

### 17.1.7 ChEMBL Target Tree

- ChEMBL

### 17.1.8 EPA CPDat Classification

- EPA Chemical and Products Database (CPDat)

### 17.1.9 Drug Enforcement Administration (DEA) Classification

- Drug Enforcement Administration (DEA)

### 17.1.10 NORMAN Suspect List Exchange Classification

- NORMAN Suspect List Exchange

### 17.1.11 EPA DSSTox Classification

- EPA DSSTox

# 18 Information Sources

FILTER BY SOURCE: ALL SOURCES

1. ## CAS Common Chemistry



*Carfentanil*

*https://commonchemistry.cas.org/detail?cas_rn=59708-52-0*

2. ## ChemIDplus



*Carfentanil [INN]*

*https://chem.nlm.nih.gov/chemidplus/sid/0059708520*

*ChemIDplus Chemical Information Classification*

*https://chem.nlm.nih.gov/chemidplus/*

3. ## DrugBank



*Carfentanil*

*https://www.drugbank.ca/drugs/DB01535*

4. ## EPA DSSTox



*Carfentanil*

*https://comptox.epa.gov/dashboard/DTXSID40208427*

*CompTox Chemicals Dashboard Chemical Lists*

*https://comptox.epa.gov/dashboard/chemical_lists/*

5. ## Hazardous Substances Data Bank (HSDB)

*Carfentanil*

*https://pubchem.ncbi.nlm.nih.gov/source/hsdb/8376*

6. ## ChEBI

*Carfentanil*

*http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:61084*

*ChEBI Ontology*

*http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology*

7. ## Drug Enforcement Administration (DEA)



*Carfentanil*

*https://www.deadiversion.usdoj.gov/schedules/*

*DEA drug and controlled substance classification*

*https://www.dea.gov/drug-scheduling*

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*https://clinicaltrials.gov/*

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http://ctdbase.org/about/legal.jsp

*http://ctdbase.org/detail.go?type=chem&acc=C017114*

10. ## Drug Gene Interaction database (DGIdb)

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The data used in DGIdb is all open access and where possible made available as raw data dumps in the downloads section.

http://www.dgidb.org/downloads

*https://www.dgidb.org/drugs/CARFENTANIL*

11. ## EPA Chemical and Products Database (CPDat)

LICENSE

https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

*https://comptox.epa.gov/dashboard/DTXSID40208427#exposure*

*EPA CPDat Classification*
*https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat*

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*LA9DTA2L8F*
*https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/*

13. ## NIST Mass Spectrometry Data Center

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https://www.nist.gov/srd/public-law

*Carfentanil*
*http://www.nist.gov/srd/nist1a.cfm*

14. ## SpectraBase

*Carfentanil*
*https://spectrabase.com/spectrum/BbxEOlWoyCO*

*Carfentanil*
*https://spectrabase.com/spectrum/FCywzXzk4w4*

*Carfentanil*
*https://spectrabase.com/spectrum/Ff9UASFfM*

*Methyl 1-phenethyl-4-(N-phenylpropionamido)piperidine-4-carboxylate*
*https://spectrabase.com/spectrum/DEZbXymPszA*

*Carfentanil*
*https://spectrabase.com/spectrum/35OJgxWJQ1o*

*Methyl 1-(2-phenylethyl)-4-(propionylanilino)-4-piperidinecarboxylate*
*https://spectrabase.com/spectrum/2voLjN6n7Ee*

*Methyl 1-(2-phenylethyl)-4-(propionylanilino)-4-piperidinecarboxylate*
*https://spectrabase.com/spectrum/7DhO2WwiDey*

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## 17. Wikipedia

*carfentanil*

***https://en.wikipedia.org/wiki/Carfentanil***

## 18. PubChem

***https://pubchem.ncbi.nlm.nih.gov***

## 19. Medical Subject Headings (MeSH)

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*carfentanil*

***https://www.ncbi.nlm.nih.gov/mesh/67017114***

*MeSH Tree*

***http://www.nlm.nih.gov/mesh/meshhome.html***

*Analgesics, Opioid*

***https://www.ncbi.nlm.nih.gov/mesh/68000701***

## 20. KEGG

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*Target-based classification of drugs*

***http://www.genome.jp/kegg-bin/get_htext?br08310.keg***

*Drug Classes*

***http://www.genome.jp/kegg-bin/get_htext?br08330.keg***

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http://www.ebi.ac.uk/Information/termsofuse.html

*Target Tree*

***https://www.ebi.ac.uk/chembl/target/browser***

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https://www.guidetopharmacology.org/about.jsp#license

*Target Classification*

***http://www.guidetopharmacology.org/***

## 23. NORMAN Suspect List Exchange

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*NORMAN Suspect List Exchange Classification*

***https://www.norman-network.com/nds/SLE/***

## 24. PATENTSCOPE (WIPO)

*SID 403470523*

***https://pubchem.ncbi.nlm.nih.gov/substance/403470523***

25. NCBI
*https://www.ncbi.nlm.nih.gov/projects/linkout*