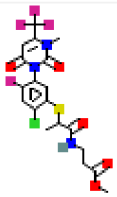
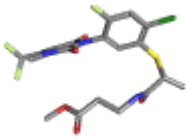
PubChem

COMPOUND SUMMARY

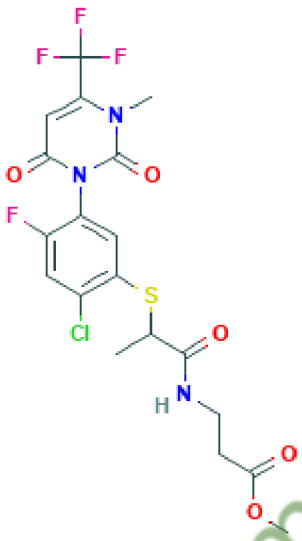
Tiafenacil

PubChem CID	67295585
Structure	 2D  3D Find Similar Structures
Chemical Safety	 Health Hazard  Environmental Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{19}H_{18}ClF_4N_3O_5S$
Synonyms	Tiafenacil 1220411-29-9 Tiafenacil [ISO] 6LL8M8V4YB methyl 3-[2-[2-chloro-4-fluoro-5-[3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]phenyl]sulfanylpropanoylamino]propanoate More...
Molecular Weight	511.9
Dates	Modify 2022-12-31 Create 2012-11-30

1 Structures

1.1 2D Structure

Chemical Structure Depiction



PubChem

1.2 3D Conformer

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

methyl 3-[2-[2-chloro-4-fluoro-5-[3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]phenyl]sulfanylpropanoylamino]propanoate

Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)

PubChem

2.1.2 InChI

InChI=1S/C19H18ClF4N3O5S/c1-9(17(30)25-5-4-16(29)32-3)33-13-7-12(11(21)6-10(13)20)27-15(28)8-14(19(22,23)24)26(2)18(27)31/h6-9H,4-5H2,1-3H3,(H,25,30)

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

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2.1.3 InChIKey

QPTPZPIXUPELRM-UHFFFAOYSA-N

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

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2.1.4 Canonical SMILES

CC(C(=O)NCCC(=O)OC)SC1=C(C=C(C(=C1)N2C(=O)C=C(N(C2=O)C)C(F)(F)F)F)Cl

Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

PubChem

2.2 Molecular Formula

C19H18ClF4N3O5S

Computed by PubChem 2.1 (PubChem release 2019.06.18)

PubChem

2.3 Other Identifiers

2.3.1 CAS

1220411-29-9

ChemIDplus; EPA DSSTox; European Chemicals Agency (ECHA); FDA Global Substance Registration System (GSRS)

2.3.2 European Community (EC) Number

868-172-7

European Chemicals Agency (ECHA)

2.3.3 UNII

6LL8M8V4YB

FDA Global Substance Registration System (GSRS)

2.3.4 DSSTox Substance ID

DTXSID20873394

EPA DSSTox

2.4 Synonyms

2.4.1 MeSH Entry Terms

methyl N-(2-((2-chloro-5-(3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl)-4-fluorophenyl) thio)-1-oxopropyl)-beta-alaninateate

tiafenacil

Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

Tiafenacil

1220411-29-9

Tiafenacil [ISO]

6LL8M8V4YB

methyl 3-[2-[2-chloro-4-fluoro-5-[3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]phenyl]sulfanylpropanoylamino]propanoate

Methyl 3-(((2RS)-2-((2-chloro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydropyrimidin-1(2H)-yl)-4-fluorophenyl)thio)propanoyl)amino)propanoate

Methyl 3-((2RS)-2-((2-chloro-5-(3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1(2H)-yl)-4-fluorophenyl)thio)propionamido)propionate

Methyl 3-(2-((2-chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydropyrimidin-1(2H)-yl)phenyl)thio)propanamido)propanoate

Methyl RAC-3-((2R)-2-((2-chloro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydropyrimidin-1(2H)-yl)-4-fluorophenyl)sulfanyl)propanamido)propanoate

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	511.9	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	2.7	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	10	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	8	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	511.0591822	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	511.0591822	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	121 Å²	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	33	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	828	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	1	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 2019.01.04)

PubChem

4 Related Records

4.1 Related Compounds with Annotation

PubChem

4.2 Related Compounds

Mixtures, Components, and Neutralized Forms	2 Records
Similar Compounds	43 Records
Similar Conformers	2 Records

PubChem

4.3 Substances

4.3.1 Related Substances

All	30 Records
Same	28 Records
Mixture	2 Records

PubChem

4.3.2 Substances by Category

- PubChem

5 Chemical Vendors

- PubChem

6 Safety and Hazards

6.1 Hazards Identification

6.1.1 GHS Classification

Pictogram(s)	 Health Hazard  Environmental Hazard
Signal	Warning
GHS Hazard Statements	H373 (100%): Causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure] H400 (100%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard] H410 (100%): Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P260, P273, P319, P391, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided by 63 companies from 1 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

▸ European Chemicals Agency (ECHA)

6.1.2 Hazard Classes and Categories

STOT RE 2 (100%)

Aquatic Acute 1 (100%)

Aquatic Chronic 1 (100%)

▸ European Chemicals Agency (ECHA)

7 Literature

7.1 NLM Curated PubMed Citations

- PubChem

7.2 Springer Nature References

- Springer Nature

7.3 Chemical Co-Occurrences in Literature

PubChem

7.4 Chemical-Gene Co-Occurrences in Literature

PubChem

7.5 Chemical-Disease Co-Occurrences in Literature

PubChem

8 Patents

8.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

8.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

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

PATENTSCOPE (WIPO)

9 Classification

9.1 MeSH Tree

- Medical Subject Headings (MeSH)

9.2 ChemIDplus

- ChemIDplus

9.3 UN GHS Classification

- UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

9.4 NORMAN Suspect List Exchange Classification

- NORMAN Suspect List Exchange

9.5 EPA DSSTox Classification

- EPA DSSTox

9.6 PFAS and Fluorinated Organic Compounds in PubChem

PubChem

9.7 EPA Substance Registry Services Tree

EPA Substance Registry Services

10 Information Sources

FILTER BY SOURCE ALL SOURCES

1. ## ChemIDplus

   LICENSE
   https://www.nlm.nih.gov/copyright.html

   Tiafenacil
   https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=1220411299

   ChemIDplus Chemical Information Classification
   https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus

2. ## EPA DSSTox

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

   Tiafenacil
   https://comptox.epa.gov/dashboard/DTXSID20873394

   CompTox Chemicals Dashboard Chemical Lists
   https://comptox.epa.gov/dashboard/chemical-lists/

3. ## European Chemicals Agency (ECHA)

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   https://echa.europa.eu/web/guest/legal-notice

   methyl 3-((2RS)-2-{2-chloro-4-fluoro-5-(1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1(6H)-yl)phenylthio}propionamido)propionate
   https://echa.europa.eu/information-on-chemicals

   methyl 3-((2RS)-2-{2-chloro-4-fluoro-5-(1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1(6H)-yl)phenylthio}propionamido)propionate
   https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/315511

4. ## FDA Global Substance Registration System (GSRS)

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   https://www.fda.gov/about-fda/about-website/website-policies#linking

   TIAFENACIL
   https://gsrs.ncats.nih.gov/ginas/app/beta/substances/6LL8M8V4YB

5. ## Springer Nature
   https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=33053112-721475452

6. ## PubChem
   https://pubchem.ncbi.nlm.nih.gov

   PFAS and Fluorinated Compounds in PubChem
   https://gitlab.lcsb.uni.lu/eci/pubchem-docs/-/raw/main/pfas-tree/PFAS_Tree.pdf?inline=false

7. ## Medical Subject Headings (MeSH)

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   https://www.nlm.nih.gov/copyright.html

   tiafenacil
   https://www.ncbi.nlm.nih.gov/mesh/2051642

   MeSH Tree

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

8. ## UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

   GHS Classification Tree
   http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

9. ## NORMAN Suspect List Exchange

   NORMAN Suspect List Exchange Classification
   https://www.norman-network.com/nds/SLE/

10. ## EPA Substance Registry Services

    EPA SRS List Classification
    https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

11. ## PATENTSCOPE (WIPO)

    SID 392695911
    https://pubchem.ncbi.nlm.nih.gov/substance/392695911