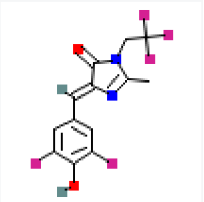
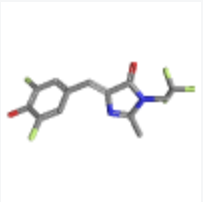
PubChem

COMPOUND SUMMARY

Dfhbi 1T

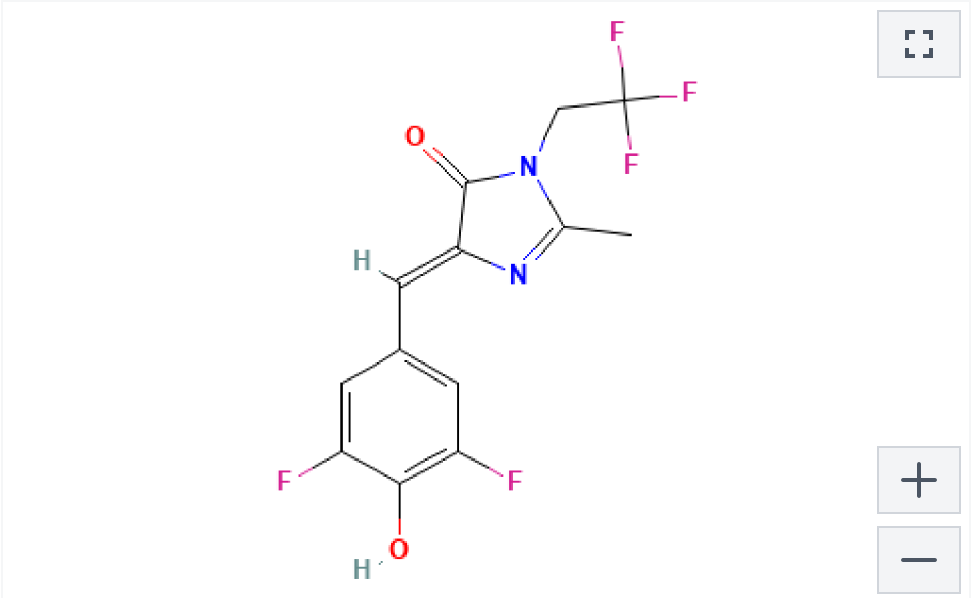
PubChem CID	101889712
Structure	 2D  3D
Molecular Formula	$C_{13}H_9F_5N_2O_2$
Synonyms	DFHBI 1T 1539318-36-9 DFHBI-1T (5Z)-5-[(3,5-Difluoro-4-hydroxyphenyl)methylene]-3,5-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-4H-imidazol-4-one (Z)-5-(3,5-Difluoro-4-hydroxybenzylidene)-2-methyl-3-(2,2,2-trifluoroethyl)-3,5-dihydro-4H-imidazol-4-one View More...
Molecular Weight	320.21 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Dates	Create: 2015-12-18 Modify: 2024-11-09

Contents

1 Structures

1.1 2D Structure

Chemical Structure Depiction



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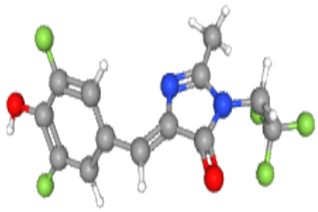
1.2 3D Conformer

Interactive Chemical Structure Model

Ball and Stick Sticks Wire-Frame Space-Filling

Show Hydrogens Animate



First Previous Conformer 1 of 9 Next Last

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

(5*Z*)-5-[(3,5-difluoro-4-hydroxyphenyl)methylidene]-2-methyl-3-(2,2,2-trifluoroethyl)imidazol-4-one

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

PubChem

2.1.2 InChI

InChI=1S/C13H9F5N2O2/c1-6-19-10(12(22)20(6)5-13(16,17)18)4-7-2-8(14)11(21)9(15)3-7/h2-4,21H,5H2,1H3/b10-4-

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

PubChem

2.1.3 InChIKey

AWYCLBWNRONMQC-WMZJFQQLSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

PubChem

2.1.4 SMILES

CC1=N/C(=C\C2=CC(=C(C(=C2)F)O)F)/C(=O)N1CC(F)(F)F

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

PubChem

2.2 Molecular Formula

$C_{13}H_9F_5N_2O_2$

Computed by PubChem 2.2 (PubChem release 2021.10.14)

PubChem

2.3 Other Identifiers

2.3.1 Nikkaji Number

J3.362.741F

Japan Chemical Substance Dictionary (Nikkaji)

2.3.2 Wikidata

Q27453430

- Wikidata

2.4 Synonyms

2.4.1 Depositor-Supplied Synonyms

DFHBI 1T
1539318-36-9
DFHBI-1T
(5Z)-5-[(3,5-Difluoro-4-hydroxyphenyl)methylene]-3,5-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-4H-imidazol-4-one
(Z)-5-(3,5-Difluoro-4-hydroxybenzylidene)-2-methyl-3-(2,2,2-trifluoroethyl)-3,5-dihydro-4H-imidazol-4-one
(5z)-5-(3,5-Difluoro-4-Hydroxybenzylidene)-2-Methyl-3-(2,2,2-Trifluoroethyl)-3,5-Dihydro-4h-Imidazol-4-One
(5Z)-5-[(3,5-difluoro-4-hydroxyphenyl)methylidene]-2-methyl-3-(2,2,2-trifluoroethyl)imidazol-4-one

- PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	320.21 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3-AA	2.5	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Hydrogen Bond Acceptor Count	8	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	320.05841834 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	320.05841834 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	52.9Å²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	22	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	505	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
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	1	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 2021.10.14)

▸ PubChem

4 Related Records

4.1 Related Compounds with Annotation

Follow these links to do a live 2D search or do a live 3D search for this compound, sorted by annotation score. This section is deprecated (see here for details), but these live search links provide equivalent functionality to the table that was previously shown here.

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4.2 Related Compounds

Same Connectivity Count	3
Same Parent, Connectivity Count	3
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

▸ PubChem

4.3 Substances

4.3.1 Related Substances

Same Count	47

▸ PubChem

4.3.2 Substances by Category

PubChem

4.4 Entrez Crosslinks

PubMed Count	1

PubChem

5 Chemical Vendors

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6 Literature

6.1 Consolidated References

PubChem

6.2 Springer Nature References

Springer Nature

6.3 Nature Journal References

Truong et al. The fluorescent aptamer Squash extensively repurposes the adenine riboswitch fold. Nature Chemical Biology, DOI: 10.1038/s41589-021-00931-2, published online 22 December 2021

Nature Chemical Biology

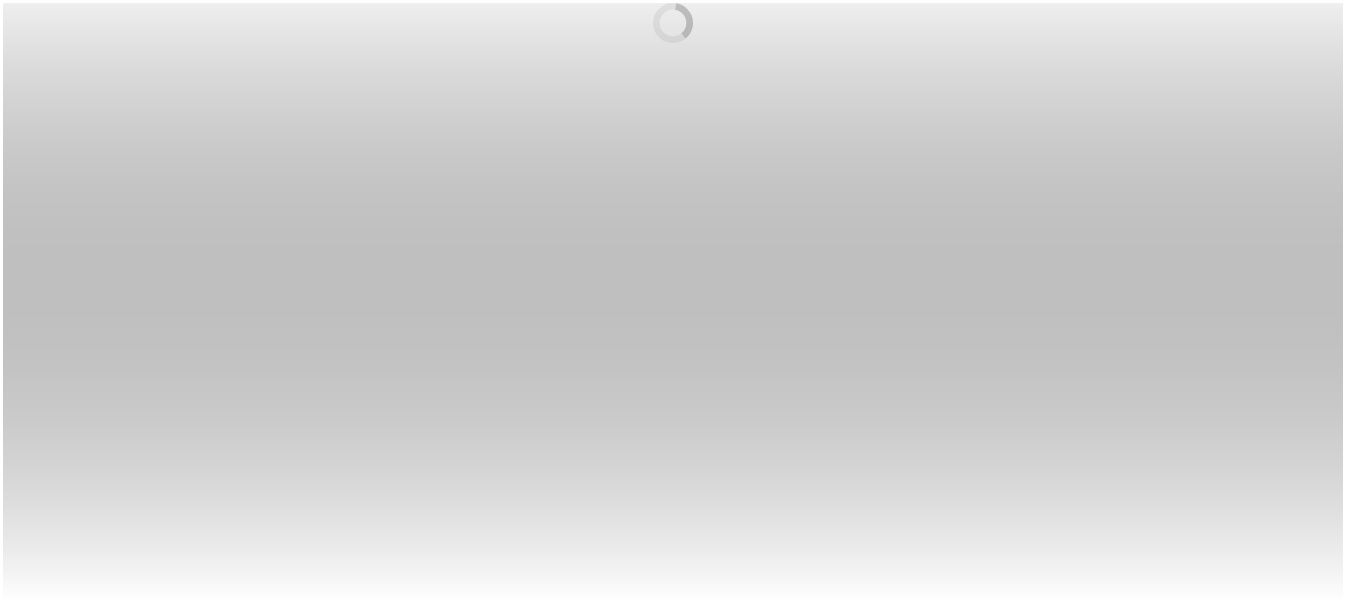
6.4 Chemical Co-Occurrences in Literature

PubChem

6.5 Chemical-Gene Co-Occurrences in Literature

PubChem

6.6 Chemical-Disease Co-Occurrences in Literature



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7 Patents

7.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

7.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

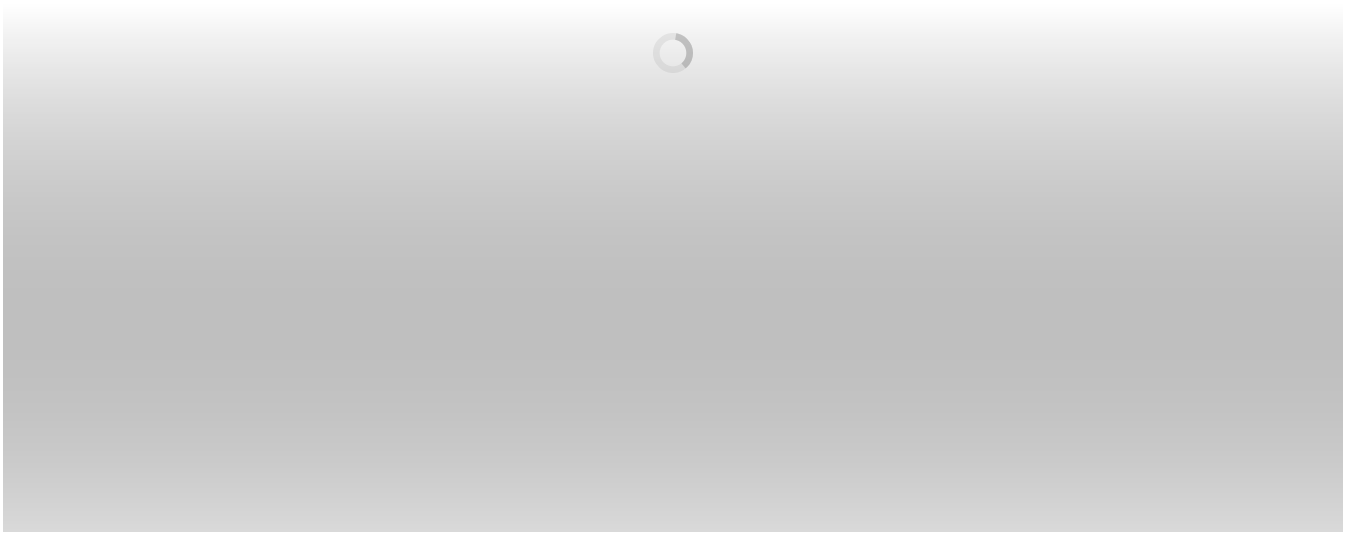
https://patentscope.wipo.int/search/en/result.jsf?inchikey=AWYCLBWNRONMQC-WMZJFQQLSA-N

▸ PATENTSCOPE (WIPO)

7.3 Chemical Co-Occurrences in Patents

▸ PubChem

7.4 Chemical-Disease Co-Occurrences in Patents



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7.5 Chemical-Gene Co-Occurrences in Patents

PubChem

8 Interactions and Pathways

8.1 Protein Bound 3D Structures

▸ RCSB Protein Data Bank (RCSB PDB)

8.1.1 Ligands from Protein Bound 3D Structures

PDBe Ligand Code	2ZY
PDBe Structure Code	4Q9R
PDBe Conformer	

▸ Protein Data Bank in Europe (PDBe)

9 Classification

9.1 PFAS and Fluorinated Organic Compounds in PubChem

PubChem

9.2 MolGenie Organic Chemistry Ontology

MolGenie

10 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. Japan Chemical Substance Dictionary (Nikkaji)

   http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J3.362.741F

2. Nature Chemical Biology

   https://pubchem.ncbi.nlm.nih.gov/substance/445509438

3. Protein Data Bank in Europe (PDBe)

   http://www.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/2ZY

4. RCSB Protein Data Bank (RCSB PDB)

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https://www.rcsb.org/pages/policies

https://www.rcsb.org/

5. ## Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=22051033-411463906

6. ## Wikidata

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(5Z)-5-(3,5-difluoro-4-hydroxybenzylidene)-2-methyl-3-(2,2,2-trifluoroethyl)-3,5-dihydro-4H-imidazol-4-one

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7. PubChem

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

PFAS and Fluorinated Compounds in PubChem

https://gitlab.com/uniluxembourg/lcsb/eci/pubchem-docs/-/raw/main/pfas-tree/PFAS_Tree.pdf?inline=false

8. ## MolGenie

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MolGenie Organic Chemistry Ontology

https://github.com/MolGenie/ontology/

9. ## PATENTSCOPE (WIPO)

SID 394163088

https://pubchem.ncbi.nlm.nih.gov/substance/394163088