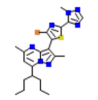
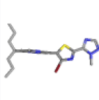




COMPOUND

3-[4-Bromo-2-(2-methyl-2H-[1,2,4]triazol-3-yl)-thiazol-5-yl]-2,5-dimethyl-7-(1-propyl-butyl)-pyrazolo[1,5-a]pyrimidine

PubChem CID	24758885
Structure	 2D  3D
Molecular Formula	C ₂₁ H ₂₆ BrN ₇ S
Synonyms	SCHEMBL2495431 RXMJMPNRLIALPQ-UHFFFAOYSA-N 3-[4-Bromo-2-(2-methyl-2H-[1,2,4]triazol-3-yl)-thiazol-5-yl]-2,5-dimethyl-7-(1-propyl-butyl)-pyrazolo[1,5-a]pyrimidine
Molecular Weight	488.4 g/mol Computed by PubChem 2.2 (PubChem release 2024.11.20)
Dates	Create: 2008-04-07 Modify: 2026-05-23

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CONTENTS

Title and Summary

1 Structures

2 Names and Identifiers

3 Chemical and Physical Properties

4 Related Records

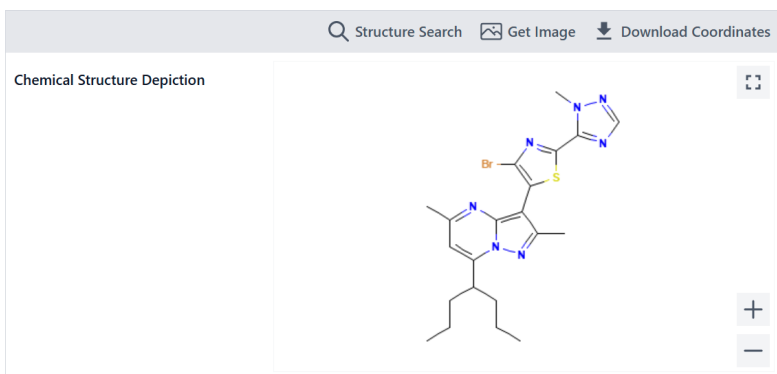
5 Patents

6 Information Sources

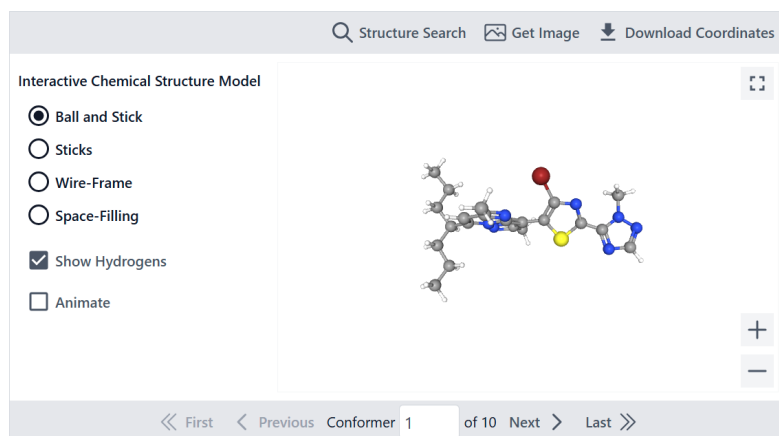
1 Structures



1.1 2D Structure

[PubChem](#)

1.2 3D Conformer



PubChem

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



4-bromo-5-(7-heptan-4-yl-2,5-dimethylpyrazolo[1,5-a]pyrimidin-3-yl)-2-(2-methyl-1,2,4-triazol-3-yl)-1,3-thiazole

Computed by Lexichem TK 2.7.0 (PubChem release 2024.11.20)

PubChem

2.1.2 InChI



InChI=1S/C₂₁H₂₆BrN₇S/c1-6-8-14(9-7-2)15-10-12(3)25-19-16(13(4)27-29(15)19)17-18(22)26-21(30-17)20-23-11-24-28(20)5/h10-11,14H,6-9H2,1-5H3

Computed by InChI 1.07.0 (PubChem release 2024.11.20)

PubChem

2.1.3 InChIKey



RXMJMPNRLIALPQ-UHFFFAOYSA-N

Computed by InChI 1.07.0 (PubChem release 2024.11.20)

PubChem

2.1.4 SMILES



CCCC(CCC)C1=CC(=NC2=C(C(=NN12)C)C3=C(N=C(S3)C4=NC=NN4C)Br)C

Computed by OEChem 2.3.0 (PubChem release 2024.12.12)

PubChem

2.2 Molecular Formula



C₂₁H₂₆BrN₇S

Computed by PubChem 2.2 (PubChem release 2024.11.20)

PubChem

2.3 Synonyms



2.3.1 Depositor-Supplied Synonyms



SCHEMBL2495431

RXMJMPNRLALPQ-UHFFFAOYSA-N

3-[4-Bromo-2-(2-methyl-2H-[1,2,4]triazol-3-yl)-thiazol-5-yl]-2,5-dimethyl-7-(1-propyl-butyl)-pyrazolo[1,5-a]pyrimidine

[PubChem](#)

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	488.4 g/mol	Computed by PubChem 2.2 (PubChem release 2024.11.20)
XLogP3-AA	5.6	Computed by XLogP3 3.0 (PubChem release 2024.11.20)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2024.11.20)
Hydrogen Bond Acceptor Count	6	Computed by Cactvs 3.4.8.18 (PubChem release 2024.11.20)
Rotatable Bond Count	7	Computed by Cactvs 3.4.8.18 (PubChem release 2024.11.20)
Exact Mass	487.11538 Da	Computed by PubChem 2.2 (PubChem release 2024.11.20)
Monoisotopic Mass	487.11538 Da	Computed by PubChem 2.2 (PubChem release 2024.11.20)
Topological Polar Surface Area	102 Å²	Computed by Cactvs 3.4.8.18 (PubChem release 2024.11.20)
Heavy Atom Count	30	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	565	Computed by Cactvs 3.4.8.18 (PubChem release 2024.11.20)
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 2019.01.04)

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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 [the neighbor discontinuation help page](#) 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 Parent, Exact Count	2
Mixtures, Components, and Neutralized Forms Count	1
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

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4.3 Substances



4.3.1 Related Substances



All Count	10
Same Count	8
Mixture Count	2

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4.3.2 Substances by Category



4 categories	Download
Curation Efforts (1)	
SureChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 228601570	External ID: SCHEMBL2495431
Governmental Organizations (1)	
PATENTSCOPE (WIPO)	
PubChem SID: 392219483	External ID: RXMJMPNRLIALPQ-UHFFFAOYSA-N
Research and Development (3)	
Google Patents	
PubChem SID: 421732692	External ID: 12905981
IBM	
PubChem SID: 245373077	External ID: 67562F8A5E1EC7A777B517B83E535AFF
SureChEMBL (Curation Efforts, Research and Development)	
PubChem SID: 228601570	External ID: SCHEMBL2495431
Legacy Depositors (4)	
DiscoveryGate (Subscription Services)	
PubChem SID: 56172674	External ID: 24758885
NextMove Software (Curation Efforts, Research and Development)	
PubChem SID: 224423184	External ID: RXMJMPNRLIALPQ-UHFFFAOYSA-N
SCRIPDB (Research and Development)	
PubChem SID: 141084511	External ID: US20100222339A1-20100902-C00018_1
Thomson Pharma (Journal Publishers, Subscription Services)	
PubChem SID: 49662710	External ID: 02544640

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5 Patents



5.1 Depositor-Supplied Patent Identifiers



36 items	Download
Search	SORT BY Priority Date - Most Recent
Methods and compositions for treating polycystic ovary syndrome Publication Number: US-11858932-B2 Priority Date: 2020-08-12 Grant Date: 2024-01-02	
Methods and compositions for treating polycystic ovary syndrome Publication Number: KR-20240023691-A Priority Date: 2020-08-12	
Methods and compositions for treating polycystic ovary syndrome Publication Number: US-12098152-B2 Priority Date: 2020-08-12 Grant Date: 2024-09-24	
Methods and compositions for treating polycystic ovary syndrome Publication Number: EP-4175572-A1 Priority Date: 2020-08-12	
Methods and compositions for treating polycystic ovary syndrome Publication Number: WO-2022036123-A1 Priority Date: 2020-08-12	
<< First < Previous Page 1 of 8 Next > Last >>	

[PubChem](#)[Link to all deposited patent identifiers](#)[PubChem](#)

5.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

<https://patentscope.wipo.int/search/en/result.jsf?inchikey=RXMJMPNRLIALPQ-UHFFFAOYSA-N>[PATENTSCOPE \(WIPO\)](#)

5.3 Chemical Co-Occurrences in Patents



Showing 3 of 100 View More Co-Occurrence and Evidence Data	Download
Chemical	Selected evidence
 3-[4-Bromo-2-(2-methyl-2H-[1,2,4]triazol-3-yl)-thiazol-5-yl]-7-(1-ethyl-propyl)-2,5-dimethyl-pyrazolo[1,5-a]pyrimidine CID 24898976	6 patents from 3 patent families View All Thiazole pyrazolopyrimidines CRF1 receptor antagonists US-8030304-B2; Grant Date: 2011-10-04
	Methods and compositions for treating polycystic ovary syndrome US-11858932-B2; Grant Date: 2024-01-02
	Methods for treating testicular and ovarian adrenal rest tumors US-11304950-B2; Grant Date: 2022-04-19
 4-(4-Chloro-5-(2,5-dimethyl-7-(pentan-3-yl)pyrazolo[1,5-a]pyrimidin-3-yl)thiazol-2-yl)morpholine	6 patents from 3 patent families View All Thiazole pyrazolopyrimidines CRF1 receptor antagonists US-8030304-B2; Grant Date: 2011-10-04
	Methods and compositions for treating polycystic ovary syndrome US-11858932-B2; Grant Date: 2024-01-02
	Methods for treating testicular and ovarian adrenal rest tumors US-11304950-B2; Grant Date: 2022-04-19

CID 24898977



4-[4-Bromo-5-(7-heptan-4-yl)-2,5-dimethylpyrazolo[1,5-a]pyrimidin-3-yl]-1,3-thiazol-2-yl)morpholine
 CID 59474059

3 patents from 1 patent family

View All [↗](#)

Thiazole pyrazolopyrimidines as crf1 receptor antagonists
 EP-2094709-B1; Grant Date: 2010-09-15

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5.4 Chemical-Disease Co-Occurrences in Patents

Showing 3 of 46 View More Co-Occurrence and Evidence Data [↗](#)

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Disease	Selected evidence
Alcoholism	3 patents from 1 patent family View All ↗ Thiazole pyrazolopyrimidines as crf1 receptor antagonists EP-2094709-B1; Grant Date: 2010-09-15
Abdominal obesity metabolic syndrome	3 patents from 1 patent family View All ↗ Thiazole pyrazolopyrimidines CRF1 receptor antagonists US-8030304-B2; Grant Date: 2011-10-04
Metabolic Syndrome	3 patents from 1 patent family View All ↗ Thiazole pyrazolopyrimidines CRF1 receptor antagonists US-8030304-B2; Grant Date: 2011-10-04

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5.5 Chemical-Gene Co-Occurrences in Patents

Showing 3 of 5 View More Co-Occurrence and Evidence Data [↗](#)

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Gene	Selected evidence
crhr1	3 patents from 1 patent family View All ↗ Thiazole pyrazolopyrimidines CRF1 receptor antagonists US-8030304-B2; Grant Date: 2011-10-04
cotl1	3 patents from 1 patent family View All ↗ Thiazole pyrazolopyrimidines CRF1 receptor antagonists US-8030304-B2; Grant Date: 2011-10-04
cgrp3	3 patents from 1 patent family View All ↗ Thiazole pyrazolopyrimidines CRF1 receptor antagonists US-8030304-B2; Grant Date: 2011-10-04

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5.6 Chemical-Organism Co-Occurrences in Patents



Showing 3 of 3 View More Co-Occurrence and Evidence Data ↗		Download
Organism	Selected evidence	
anseriformes (ducks, geese & swans)	2 patents from 1 patent family View All ↗	
	Thiazole pyrazolopyrimidines CRF1 receptor antagonists US-8030304-B2; Grant Date: 2011-10-04	
rattus (rats)	3 patents from 1 patent family View All ↗	
	Thiazole pyrazolopyrimidines CRF1 receptor antagonists US-8030304-B2; Grant Date: 2011-10-04	
metazoa (animals)	3 patents from 1 patent family View All ↗	
	Thiazole pyrazolopyrimidines CRF1 receptor antagonists US-8030304-B2; Grant Date: 2011-10-04	

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6 Information Sources



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1. PubChem

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

2. PATENTSCOPE (WIPO)

SID 392219483

<https://pubchem.ncbi.nlm.nih.gov/substance/392219483>

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