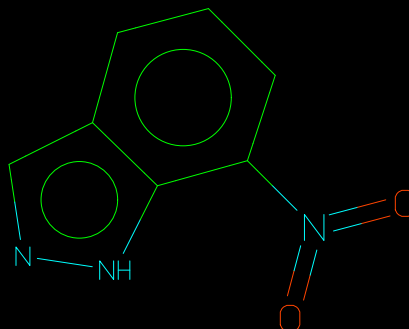


SMILES

Fingerprint	256 bytes of binary data
Orig nbits	2048
Orig nbits set	124
Nbits	2048
Nbits set	124
Version	4.72
ID	VCS_model

Parent Avg molecular weight	163.15
------------------------------------	--------

Parent Molecular Formula	C7H5N3O2
---------------------------------	----------

Parent rotatable bond count	1
------------------------------------	---

Parent H-bond donor count	1
----------------------------------	---

Parent H-bond acceptor count	5
-------------------------------------	---

Parent accurate mass	163.038177
-----------------------------	------------

Parent ring count	2
--------------------------	---

Parent Rigidity	0.7500
------------------------	--------

Parent Fragment count	2
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Parent part count	1
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Parent polar surface area	74.50
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Timestamp	200108210415.23
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Graph	ON(O)C1CCCC2CNNC21
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SMILES O=N(=O)c1cccc2cn[nH]c12

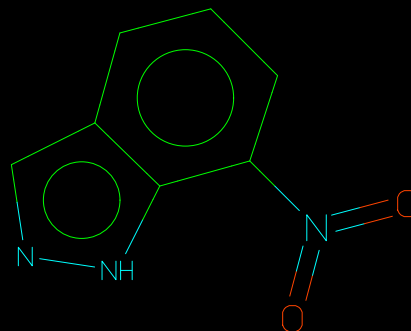
Supplier's Primary Identifier

N163

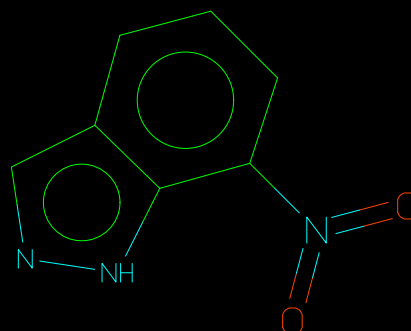
Supplier/Collection

lopac

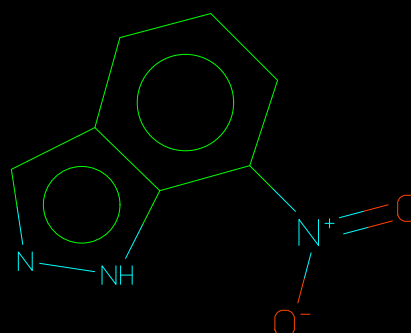
Parent Isomeric SMILES



Normalised Version Isomeric SMILES



Version Isomeric SMILES



Version 2D-coordinates

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Comment

Version coordinates

SMILES O=N(=O)c1cccc2cn[nH]c12

Supplier's Primary Identifier

Fingerprint of version

256 bytes of binary data
Orig nbits 2048
Orig nbits set 141
Nbits 2048
Nbits set 141
Version 4.72
ID VCS_model

Version Avg molecular weight
163.15

Version Molecular Formula
C7H5N3O2

Data_type ID
Value 453

Data_type CATNUM
Value N-163

Data_type NAME
Value 7-Nitroindazole

Supplier's Seconadary Identifier
7NITROINDAZOLE

Data_type POSITION
Value RK006-F8

Data_type ACTION
Value Inhibitor

Data_type CLASS
Value Enzyme

Data_type SELECTIVITY
Value bNOS

Data_type DESCRIPTION
Value Selective inhibitor of brain nitric oxide synthase

Supplier/Collection
rbi

Version 2D-coordinates
3.21,-0.15,2.35,-0.65,1.48,-0.15,2.35,-1.65,1.50,-2.18,1.50,-3.18,2.35,-3.66,3.20,-3.13,4.98,-3.17,4.98,-2.17,4.12,-1.67,3.20,-2.12

Comment Version coordinates

Data_type POSITION
Value RK006-E8

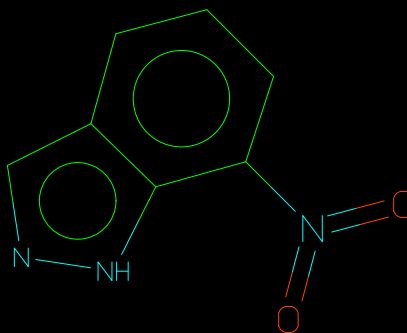
Supplier's Primary Identifier
AG376/4246

SMILES O=N(=O)c1cccc2cn[nH]c12

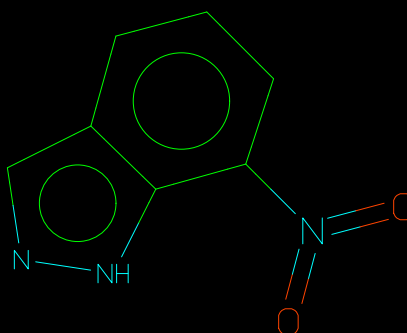
Supplier's Primary Key 10701246

Supplier/Collection
specs

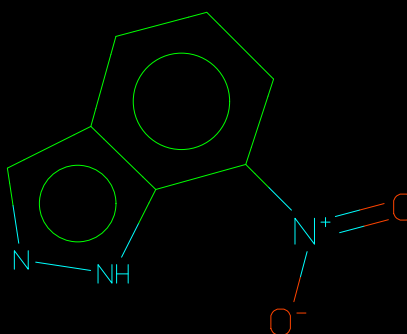
Parent Isomeric SMILES



Normalised Version Isomeric SMILES



Version Isomeric SMILES



Version 2D-coordinates

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Comment

Version coordinates

SMILES O=N(=O)c1cccc2cn[nH]c12

Supplier's Primary Identifier
AG-376/4246

Fingerprint of version

256 bytes of binary data
Orig nbits 2048
Orig nbits set 141
Nbits 2048
Nbits set 141
Version 4.72
ID VCS_model

Version Avg molecular weight
163.15

Version Molecular Formula
C7H5N3O2

Data_type ISISUNIQUEID
Value 1003

Data_type CIFNUMBER
Value CIF4246

Data_type AMOUNT_0
Value 100 mg

Data_type USES
Value Potent and selctive inhibitor of cerebella nitric oxide synthase

Data_type IDNUMBER
Value AG-376/4246

Data_type PRICE
Value Y

Data_type CAS_NO_
Value 002942-42-9

Supplier's Seconadary Identifier
002942429

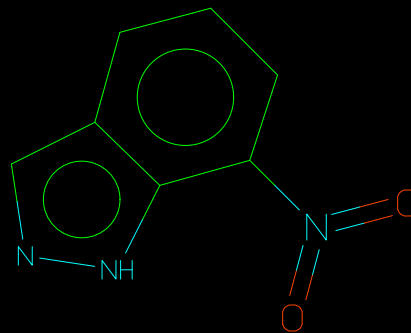
Supplier's Primary Identifier
0602

Supplier/Collection
tocris

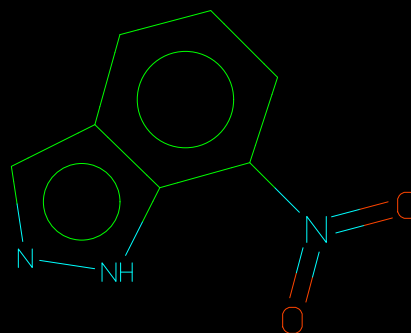
SMILES O=N(=O)c1cccc2cn[nH]c12

Supplier's Primary Identifier

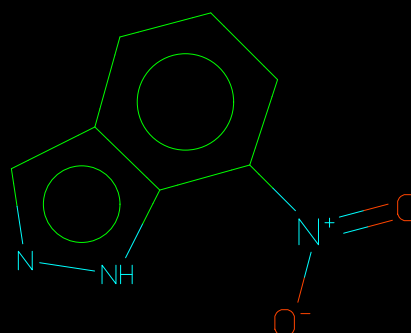
Parent Isomeric SMILES



Normalised Version Isomeric SMILES



Version Isomeric SMILES



Version 2D-coordinates

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Comment

Version coordinates

SMILES O=N(=O)c1cccc2cn[nH]c12

Supplier's Primary Identifier

Fingerprint of version

256 bytes of binary data
Orig nbits 2048
Orig nbits set 141
Nbits 2048
Nbits set 141
Version 4.72
ID VCS_model

Version Avg molecular weight
163.15

Version Molecular Formula
C7H5N3O2

Data_type CATALOGUE_NO
Value 0602

Data_type COMPOUND_NAME
Value 7-Nitroindazole

Supplier's Secondary Identifier
7NITROINDAZOLE

Supplier/Collection
tocris2000

Data_type CATEGORY
Value Nitric Oxide Compound

Data_type ACTION
Value Prototypical selective nNOS inhibitor

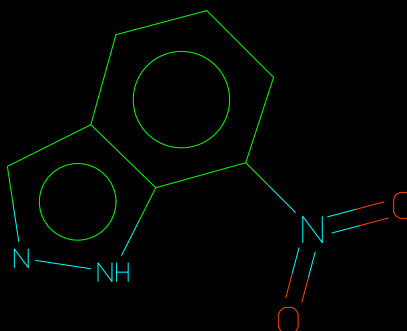
Supplier/Collection
tocris2001

Supplier's Primary Identifier

0800

Supplier/Collection
tocris

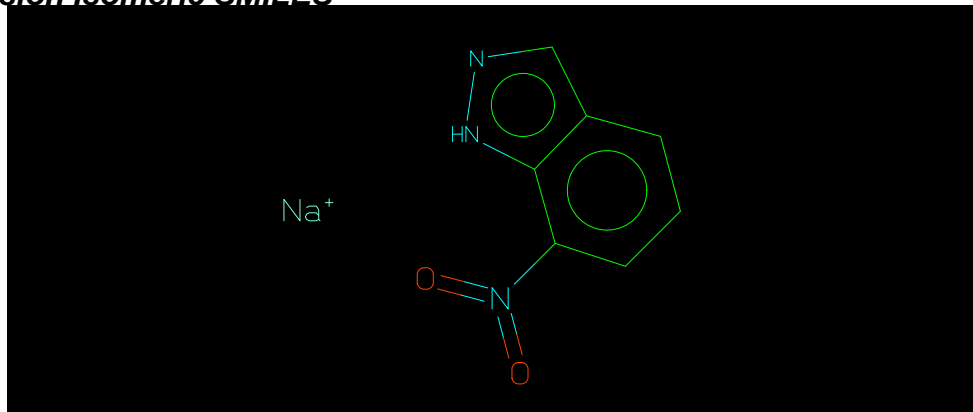
Parent Isomeric SMILES



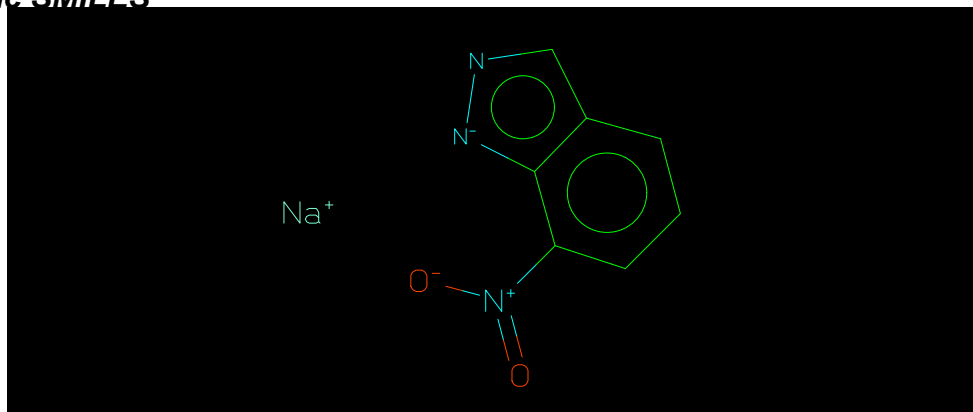
SMILES O=N(=O)c1cccc2cn[nH]c12

Supplier's Primary Identifier 0800

Normalised Version Isomeric SMILES



Version Isomeric SMILES



Version 2D-coordinates

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Comment Version coordinates

Fingerprint of version

256 bytes of binary data

Orig nbits 2048

Orig nbits set 144

Nbits 2048

Nbits set 144

Version 4.72

ID VCS_model

Version Avg molecular weight

22.99,162.14

Version Molecular Formula

Na,C₇H₄N₃O₂

Data_type CATALOGUE_NO

Value 0800

SMILES	O=N(=O)c1cccc2cn[nH]c12
Supplier's Primary Identifier	
Data_type	COMPOUND_NAME
Value	7-Nitroindazole monosodium salt
Supplier's Secondary Identifier	
	7NITROINDAZOLEMONOSODIUMSALT
Supplier/Collection	
	tocris2000
Data_type	CATEGORY
Value	Nitric Oxide Compound
Data_type	ACTION
Value	Water soluble sodium salt of (0602)
Supplier/Collection	
	tocris2001
Data_type	COMPOUND_NAME
Value	7-NINA
Supplier's Secondary Identifier	
	7NINA