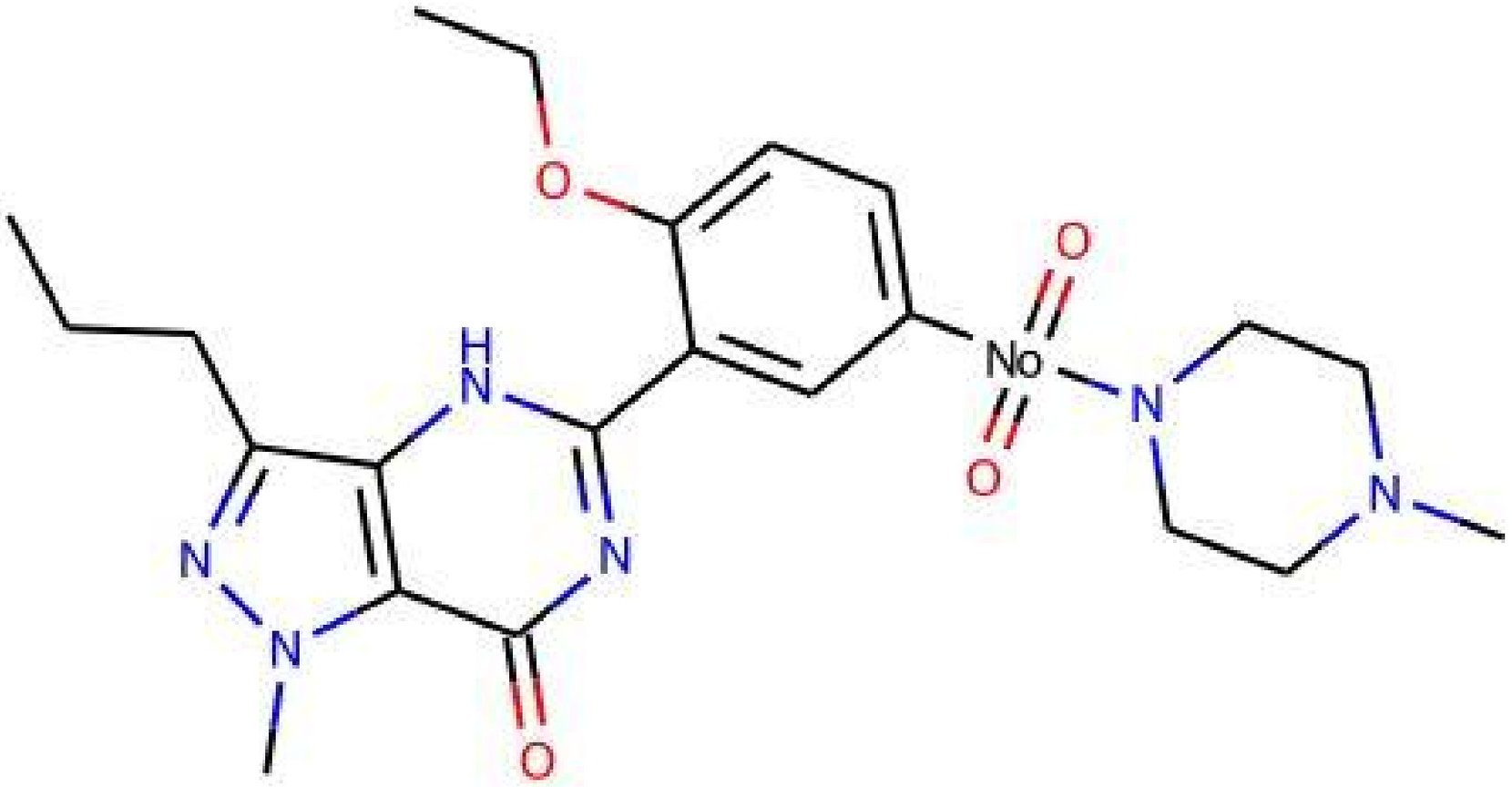
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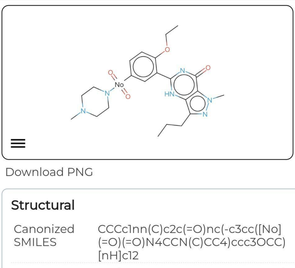

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Structural

Canonized SMILES	CCCc1nn(C)c2c(=O)nc(-c3cc([No](=O)(=O)N4CCN(C)CC4)ccc3OCC)[nH]c12
InChI	InChI=1S/C17H19N4O2.C5H11N2.No.2O/c1-4-8-12-14-15(21(3)20-12)17(22)19-16(18-14)11-9-6-7-10-13(11)23-5-2;1-7-4-2-6-3-5-7;;;;/h7,9-10H,4-5,8H2,1-3H3,(H,18,19,22);2-5H2,1H3;;;/q;-1;+1;;
InChI key	LVHPOVVKVZTLEJ-UHFFFAOYSA-N
IUPAC name	
Chemical formula	$C_{22}H_{30}N_6NoO_4$
Molecular weight	701.52

Bio

CYP1A2	Noninhibitor
CYP2C19	Noninhibitor
CYP2C9	Noninhibitor
CYP2D6	Noninhibitor
CYP3A4	Noninhibitor

Physical

Water Solubility	-3.9 LogS
Water Solubility (QSAR)	-4.27 ± 0.23 Log(mol/L)
Vapor Pressure	-8.1 log(mmHg)
Vapor Pressure (QSAR)	8.2 ± 9.8 Torr
Boiling point	398 Celsius
Boiling point (QSAR)	155 ± 24 °C
Flash point	390 Celsius
Density	1.98 g/cm3
Density (QSAR)	1.324 ± 0.02 g/cm3
Density (normal) (QSAR)	1.299 ± 0.03 g/cm3
Viscosity	1.1 log10(viscosity cP)
Melting point	220 Celsius
Melting point (QSAR)	206 ± 6 °C
LogP octanol-water	0.9 logP
Soluble in DMSO	Soluble
DMSO Solubility (QSAR)	0.44 ± 0.06 (Undefined)
Retention time	510 s
Retention time (QSAR)	638 ± 12 s
Refractive Index (QSAR)	1.526 ± 0.012

Toxicity

Developmental toxicity	Positive	
Mouse Intravenous	910 mg/kg	
Rat Oral	5131 mg/kg	
Rabbit Intravenous	407 mg/kg	
Rat Intravenous	1007 mg/kg	
Mouse Intraperitoneal LD50	913 mg/kg	from: 798 to: 1045
Mouse Intravenous LD50	212 mg/kg	from: 188 to: 239
Mouse Intraperitoneal LDLo	881 mg/kg	from: 731 to: 1062
Rat Intraperitoneal LD50	786 mg/kg	from: 626 to: 986
Mouse Oral LD50	3039 mg/kg	from: 2763 to: 3342
Mouse Subcutaneous LD50	1190 mg/kg	from: 967 to: 1463
Rat Subcutaneous LD50	716 mg/kg	from: 585 to: 877
Mouse Unreported LDLo	993 mg/kg	from: 832 to: 1184
Rat Unreported LD50	2304 mg/kg	from: 1898 to: 2798
Mouse Unreported LD50	1479 mg/kg	from: 1187 to: 1844
Rat Intraperitoneal LDLo	503 mg/kg	from: 401 to: 632
Rabbit Skin LD50	3989 mg/kg	from: 3273 to: 4861
Rat Oral LD50	2599 mg/kg	from: 2210 to: 3056
Rat Oral LDLo	1147 mg/kg	from: 947 to: 1391
Rabbit Oral LD50	2314 mg/kg	from: 1925 to: 2783
Rabbit Intravenous LD50	66 mg/kg	from: 53 to: 81
Rat Intravenous LD50	168 mg/kg	from: 136 to: 208
Mouse Oral LDLo	1720 mg/kg	from: 1472 to: 2008
Rat Skin LD50	4319 mg/kg	from: 3850 to: 4844
Mammal (species unspecified) Subcutaneous LD50	1016 mg/kg	from: 895 to: 1154
Guinea Pig Oral LD50	1067 mg/kg	from: 816 to: 1397

Ecology

Bioconcentration factor	1.1 Log10(BCF)
Bioconcentration factor (QSAR)	1.3 ± 0.1 Log(L/kg)
40 hour Tetrahymena pyriformis IGC50	4 Log10 (IGC50 mol/L)
48 hour Daphnia magna LC50	7.1 Log10 (LC50 mol/L)

Mutagenicity

Ames test	Negative
Ames test (QSAR)	0.44 ± 0.14 (Undefined)

Synthesis

SYBA	50.24
Complexity	4,76

Drug-likeness

Lipinski's rule of five

Hydrogen bond donors <= 5	1 donors
Hydrogen bond acceptors <= 10	10 acceptors
Molecular weight < 500	701.52 g/mol
LogP octanol-water <= 5	0.9 logP

Ghose filter

LogP octanol-water [-0.4, 5.6]	0.9 logP
Molecular weight [180, 480]	701.52 g/mol
Number of atoms [20, 70]	33 atoms
Molar refractivity [40, 130]	119.81 m3/mol

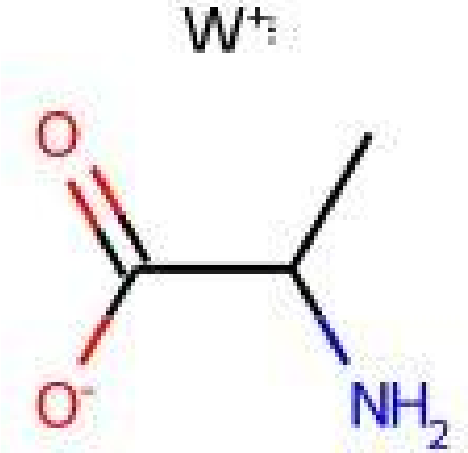
Oprea's Rule

Hydrogen bond donors <= 2	1 donors
Hydrogen bond acceptors [2, 9]	10 acceptors
Number of rotatable bonds [2, 8]	7 bonds
Number of rings [1, 4]	1 rings

Veber's Rule

Hydrogen bond donors <= 2	7 bonds
TPSA <= 140 Å²	113.42 Å²

QED - quantitative estimate of drug-likeness	0.39
Topological polar surface area (including sulphur and phosphorus)	113.42 Å²
PAINS	not included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O-
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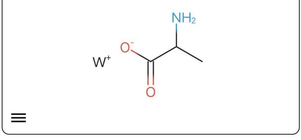

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Structural

Canonized SMILES	CC(N)C(=O)[O-].[W+]
InChI	InChI=1S/C3H7NO2.W/c1-2(4)3(5)6;/h2H,4H2,1H3,(H,5,6);/q;+1/p-1
InChI key	KVJYAIUIECNNRA-UHFFFAOYSA-M
IUPAC name	2-aminopropanoyloxytungsten
Chemical formula	$C_3H_6NO_2W$
Molecular weight	271.926

Bio

CYP1A2	Noninhibitor
CYP2C19	Inhibitor
CYP2C9	Inhibitor
CYP2D6	Noninhibitor
CYP3A4	Noninhibitor

Physical

Water Solubility	-0.8 LogS
Water Solubility (QSAR)	-0.17 ± 0.1 Log(mol/L)
Vapor Pressure	-1.1 log(mmHg)
Vapor Pressure (QSAR)	30.8 ± 12 Torr
Boiling point	177 Celsius
Boiling point (QSAR)	160 ± 9 °C
Flash point	80 Celsius
Density	1.67 g/cm3
Density (QSAR)	2.247 ± 0.085 g/cm3
Density (normal) (QSAR)	2.049 ± 0.053 g/cm3
Viscosity	0.4 log10(viscosity cP)
Melting point	140 Celsius
Melting point (QSAR)	178 ± 16 °C
LogP octanol-water	-2 logP
Soluble in DMSO	Soluble
DMSO Solubility (QSAR)	1 0 (Soluble)
Retention time	280 s
Retention time (QSAR)	438 ± 76 s
Refractive Index (QSAR)	1.46 ± 0.006

Toxicity

Developmental toxicity	Positive	
Mouse Intravenous	null mg/kg	
Rat Oral	0.00 mg/kg	
Rabbit Intravenous	null mg/kg	
Rat Intravenous	null mg/kg	
Mouse Intraperitoneal LD50	1414 mg/kg	from: 1089 to: 1835
Mouse Intravenous LD50	916 mg/kg	from: 717 to: 1169
Mouse Intraperitoneal LDLo	1545 mg/kg	from: 1229 to: 1941
Rat Intraperitoneal LD50	1905 mg/kg	from: 1477 to: 2456
Mouse Oral LD50	3285 mg/kg	from: 2499 to: 4318
Mouse Subcutaneous LD50	5352 mg/kg	from: 3982 to: 7195
Rat Subcutaneous LD50	3889 mg/kg	from: 3096 to: 4886
Mouse Unreported LDLo	963 mg/kg	from: 690 to: 1343
Rat Unreported LD50	2793 mg/kg	from: 2160 to: 3612
Mouse Unreported LD50	3083 mg/kg	from: 2398 to: 3964
Rat Intraperitoneal LDLo	1266 mg/kg	from: 952 to: 1683
Rabbit Skin LD50	9027 mg/kg	from: 7008 to: 11629
Rat Oral LD50	4849 mg/kg	from: 3737 to: 6291
Rat Oral LDLo	3313 mg/kg	from: 2450 to: 4481
Rabbit Oral LD50	3083 mg/kg	from: 2383 to: 3989
Rabbit Intravenous LD50	833 mg/kg	from: 629 to: 1102
Rat Intravenous LD50	1503 mg/kg	from: 1117 to: 2021
Mouse Oral LDLo	2450 mg/kg	from: 1906 to: 3150
Rat Skin LD50	6741 mg/kg	from: 5518 to: 8237
Mammal (species unspecified) Subcutaneous LD50	2228 mg/kg	from: 1739 to: 2856
Guinea Pig Oral LD50	2988 mg/kg	from: 2268 to: 3937

Ecology

Bioconcentration factor	0.3 Log10(BCF)
Bioconcentration factor (QSAR)	0.7 ± 0.1 Log(L/kg)
40 hour Tetrahymena pyriformis IGC50	3.2 Log10 (IGC50 mol/L)
48 hour Daphnia magna LC50	4.4 Log10 (LC50 mol/L)

Mutagenicity

Ames test	Negative
Ames test (QSAR)	0.6 ± 0.11 (Positive)

Synthesis

SYBA	8.91
Complexity	1

Drug-likeness

Lipinski's rule of five

Hydrogen bond donors <= 5	2 donors
Hydrogen bond acceptors <= 10	3 acceptors
Molecular weight < 500	271.93 g/mol
LogP octanol-water <= 5	-2 logP

Ghose filter

LogP octanol-water [-0.4, 5.6]	-2 logP
Molecular weight [180, 480]	271.93 g/mol
Number of atoms [20, 70]	7 atoms
Molar refractivity [40, 130]	18.66 m3/mol

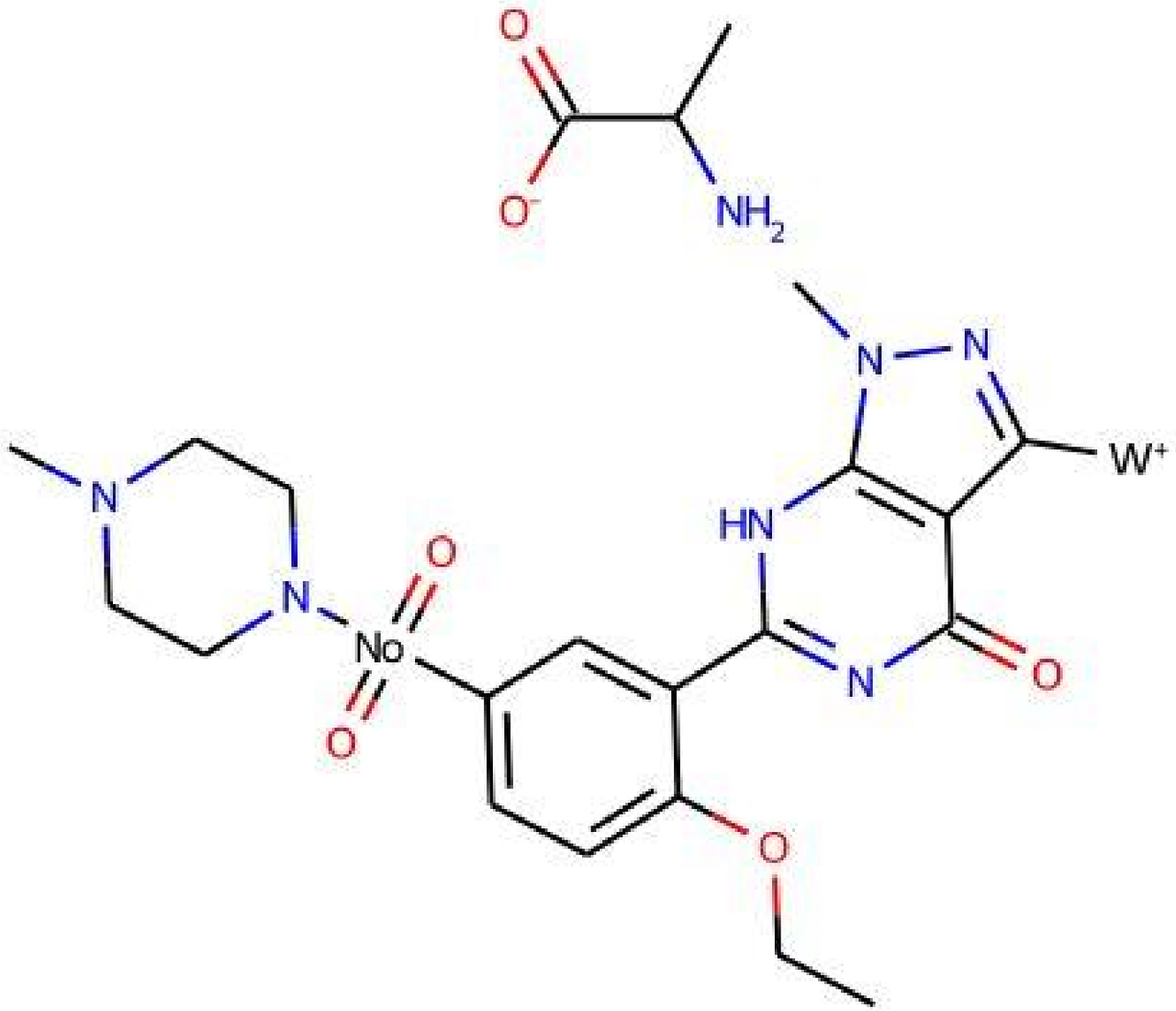
Oprea's Rule

Hydrogen bond donors <= 2	2 donors
Hydrogen bond acceptors [2, 9]	3 acceptors
Number of rotatable bonds [2, 8]	1 bonds
Number of rings [1, 4]	2 rings

Veber's Rule

Hydrogen bond donors <= 2	1 bonds
TPSA <= 140 Å²	66.15 Å²

QED - quantitative estimate of drug-likeness	0.6
Topological polar surface area (including sulphur and phosphorus)	66.15 Å²
PAINS	not included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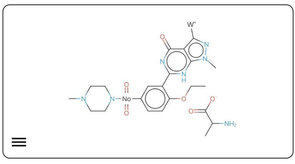

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Structural

Canonized SMILES	CC(N)C(=O)[O-].CCOc1ccc([No](=O)(=O)N2CCN(C)CC2)cc1-c1nc(=O)c2c([W+])nn(C)c2[nH]1
InChI	InChI=1S/C14H12N4O2.C5H11N2.C3H7NO2.No.2O.W/c1-3-20-11-7-5-4-6-9(11)12-16-13-10(14(19)17-12)8-15-18(13)2;1-7-4-2-6-3-5-7;1-2(4)3(5)6;;;;;/h5-7H,3H2,1-2H3,(H,16,17,19);2-5H2,1H3;2H,4H2,1H3,(H,5,6);;;;;/q;-1;;+1;;;+1/p-1
InChI key	AFIZFDRIGVVASK-UHFFFAOYSA-M
IUPAC name	
Chemical formula	$C_{22}H_{29}N_7NoO_6W$
Molecular weight	930.357

Bio

CYP1A2	Noninhibitor
CYP2C19	Noninhibitor
CYP2C9	Inhibitor
CYP2D6	Noninhibitor
CYP3A4	Noninhibitor

Physical

Water Solubility	-1.7 LogS
Water Solubility (QSAR)	-3.76 ± 0.17 Log(mol/L)
Vapor Pressure	-7.5 log(mmHg)
Vapor Pressure (QSAR)	12.1 ± 9.1 Torr
Boiling point	312 Celsius
Boiling point (QSAR)	127 ± 24 °C
Flash point	420 Celsius
Density	2.03 g/cm3
Density (QSAR)	1.64 ± 0.051 g/cm3
Density (normal) (QSAR)	1.657 ± 0.032 g/cm3
Viscosity	1.3 log10(viscosity cP)
Melting point	250 Celsius
Melting point (QSAR)	215 ± 7 °C
LogP octanol-water	-0.4 logP
Soluble in DMSO	Soluble
DMSO Solubility (QSAR)	0.5 ± 0.05 (Soluble)
Retention time	340 s
Retention time (QSAR)	609 ± 6 s
Refractive Index (QSAR)	1.533 ± 0.007

Toxicity

Developmental toxicity	Positive
Mouse Intravenous	null mg/kg
Rat Oral	0.00 mg/kg
Rabbit Intravenous	null mg/kg
Rat Intravenous	null mg/kg
Mouse Intraperitoneal LD50	1589 mg/kg (from: 1405 to: 1798)
Mouse Intravenous LD50	781 mg/kg (from: 619 to: 986)
Mouse Intraperitoneal LDLo	1537 mg/kg (from: 1251 to: 1889)
Rat Intraperitoneal LD50	1599 mg/kg (from: 1317 to: 1942)
Mouse Oral LD50	6703 mg/kg (from: 5627 to: 7983)
Mouse Subcutaneous LD50	1914 mg/kg (from: 1563 to: 2343)
Rat Subcutaneous LD50	1505 mg/kg (from: 1150 to: 1970)
Mouse Unreported LDLo	2244 mg/kg (from: 1656 to: 3040)
Rat Unreported LD50	4249 mg/kg (from: 3495 to: 5164)
Mouse Unreported LD50	3461 mg/kg (from: 2941 to: 4072)
Rat Intraperitoneal LDLo	1219 mg/kg (from: 1015 to: 1464)
Rabbit Skin LD50	8137 mg/kg (from: 6162 to: 10744)
Rat Oral LD50	6385 mg/kg (from: 4993 to: 8165)
Rat Oral LDLo	3338 mg/kg (from: 2527 to: 4408)
Rabbit Oral LD50	5541 mg/kg (from: 4340 to: 7073)
Rabbit Intravenous LD50	217 mg/kg (from: 166 to: 283)
Rat Intravenous LD50	786 mg/kg (from: 602 to: 1027)
Mouse Oral LDLo	3801 mg/kg (from: 3154 to: 4579)
Rat Skin LD50	10087 mg/kg (from: 8080 to: 12592)
Mammal (species unspecified) Subcutaneous LD50	1408 mg/kg (from: 1194 to: 1660)
Guinea Pig Oral LD50	3978 mg/kg (from: 2759 to: 5735)

Ecology

Bioconcentration factor	1.1 Log10(BCF)
Bioconcentration factor (QSAR)	1 ± 0.1 Log(L/kg)
40 hour Tetrahymena pyriformis IGC50	3.7 Log10 (IGC50 mol/L)
48 hour Daphnia magna LC50	7 Log10 (LC50 mol/L)

Mutagenicity

Ames test	Negative
Ames test (QSAR)	0.91 ± 0.08 (Positive)

Synthesis

SYBA	36.35
Complexity	4.45

Drug-likeness

Lipinski's rule of five

Hydrogen bond donors <= 5	3 donors
Hydrogen bond acceptors <= 10	13 acceptors
Molecular weight < 500	930.36 g/mol
LogP octanol-water <= 5	-0.4 logP

Ghose filter

LogP octanol-water [-0.4, 5.6]	-0.4 logP
Molecular weight [180, 480]	930.36 g/mol
Number of atoms [20, 70]	37 atoms
Molar refractivity [40, 130]	124.1 m3/mol

Oprea's Rule

Hydrogen bond donors <= 2	3 donors
Hydrogen bond acceptors [2, 9]	13 acceptors
Number of rotatable bonds [2, 8]	6 bonds
Number of rings [1, 4]	3 rings

Veber's Rule

Hydrogen bond donors <= 2	6 bonds
TPSA <= 140 Å²	179.57 Å²

QED - quantitative estimate of drug-likeness	0.27
Topological polar surface area (including sulphur and phosphorus)	179.57 Å²
PAINS	not included