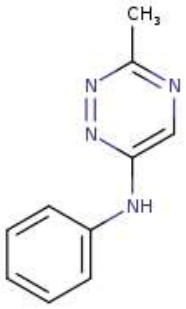
Molecule 1



SMILES Cc1ncc(nn1)Nc1ccccc1

Physicochemical Properties	
Formula	C10H10N4
Molecular weight	186.21 g/mol
Num. heavy atoms	14
Num. arom. heavy atoms	12
Fraction Csp3	0.10
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	1
Molar Refractivity	54.34
TPSA	50.70 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.84
Log $P_{o/w}$ (XLOGP3)	1.47
Log $P_{o/w}$ (WLOGP)	1.92
Log $P_{o/w}$ (MLOGP)	1.34
Log $P_{o/w}$ (SILICOS-IT)	1.62
Consensus Log $P_{o/w}$	1.64

Water Solubility	
Log *S* (ESOL)	-2.42
Solubility	7.03e-01 mg/ml ; 3.78e-03 mol/l
Class	Soluble
Log *S* (Ali)	-2.14
Solubility	1.34e+00 mg/ml ; 7.22e-03 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-4.24
Solubility	1.08e-02 mg/ml ; 5.79e-05 mol/l
Class	Moderately soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-6.39 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: MW<200
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	2.60