SwissADME

This website allows you to compute physicochemical descriptors as well as to predict ADME parameters, pharmacokinetic properties, druglike nature and medicinal chemistry friendliness of one or multiple small molecules to support drug discovery.

The main article describing the web service and its underlying methodologies is SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Sci. Rep.* (2017) 7:42717.
For details about development and validation of iLOG, please refer to this article: iLOGP: a simple, robust, and efficient description of *n*-octanol/water partition coefficient for drug design using the GB/SA approach. *J. Chem. Inf. Model.* (2014) 54(12):3284-3301.
For details about development and validation of the BOILED-Egg, please refer to this article: A BOILED-Egg to predict gastrointestinal absorption and brain penetration of small molecules. *ChemMedChem* (2016) 11(11):1117-1121.

Developed and maintained by the Molecular Modeling Group of the SIB | Swiss Institute of Bioinformatics.

Enter a list of SMILES here:

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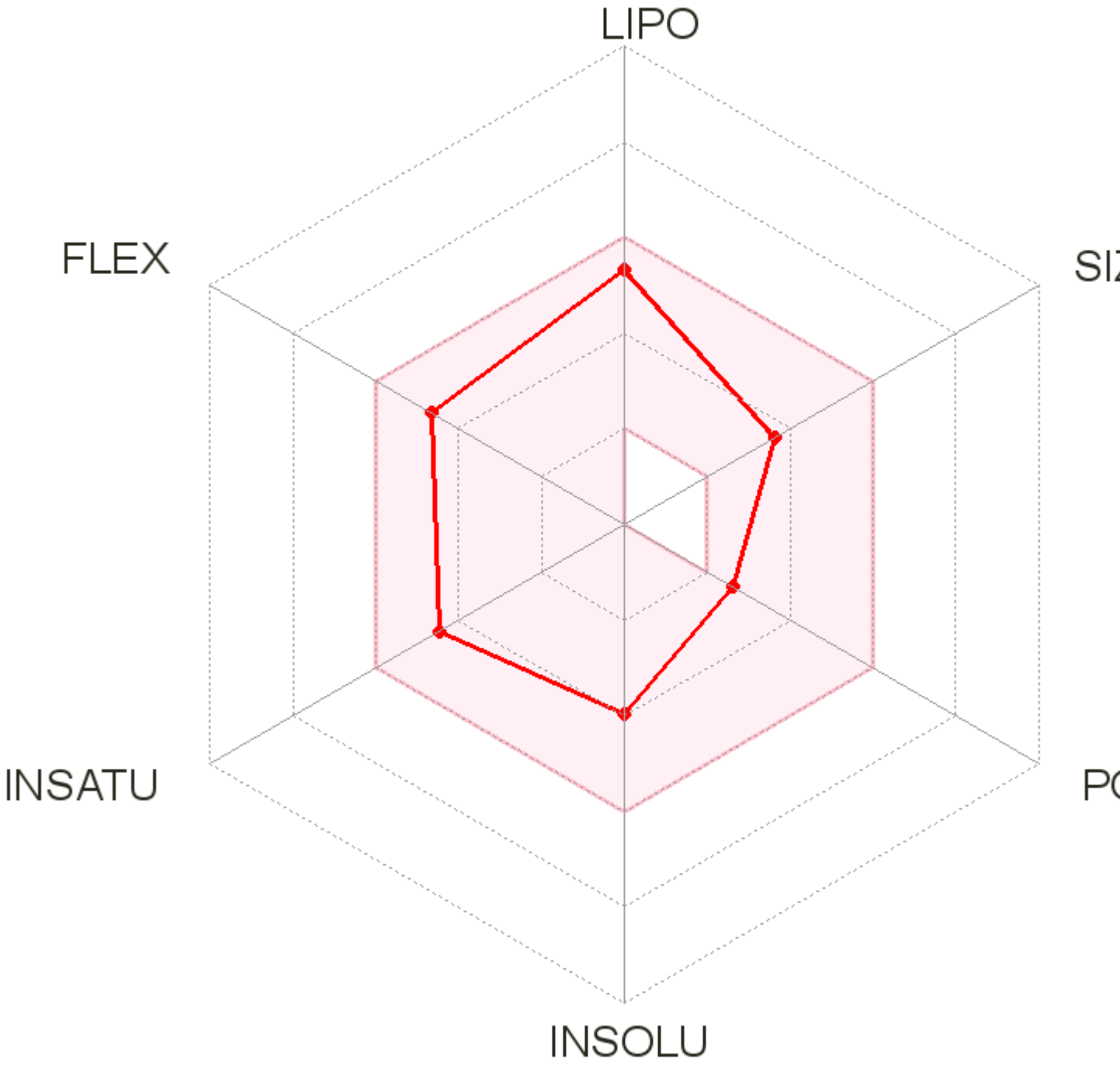
Molecule 1



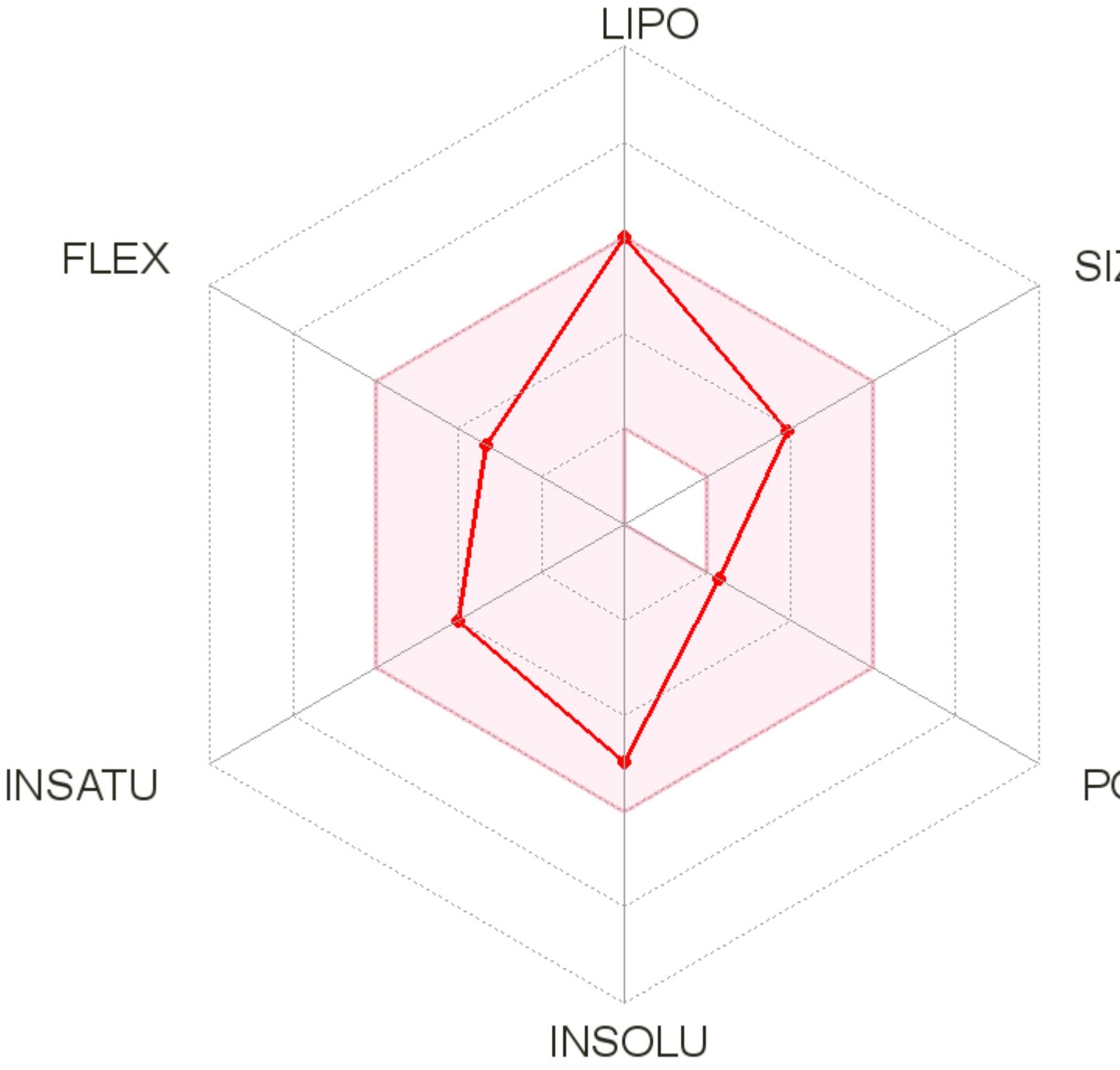
SMILES CCNCCCC(Nc1ccnc2c1ccc(c2)Cl)C

Physicochemical Properties

Formula	C16H22ClN3
Molecular weight	291.82 g/mol
Num. heavy atoms	20
Num. arom. heavy atoms	10
Fraction Csp3	0.44
Num. rotatable bonds	7
Num. H-bond acceptors	2
Num. H-bond donors	2
Molar Refractivity	87.70
TPSA	36.95 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.43
Log $P_{o/w}$ (XLOGP3)	3.80
Log $P_{o/w}$ (WLOGP)	3.89
Log $P_{o/w}$ (MLOGP)	2.73
Log $P_{o/w}$ (SILICOS-IT)	3.98
Consensus Log $P_{o/w}$	3.57
Water Solubility	
Log *S* (ESOL)	-3.95
Solubility	3.26e-02 mg/ml ; 1.12e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.27
Solubility	1.57e-02 mg/ml ; 5.37e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-6.86
Solubility	4.07e-05 mg/ml ; 1.40e-07 mol/l
Class	Poorly soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes

CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-5.38 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.54

Molecule 2



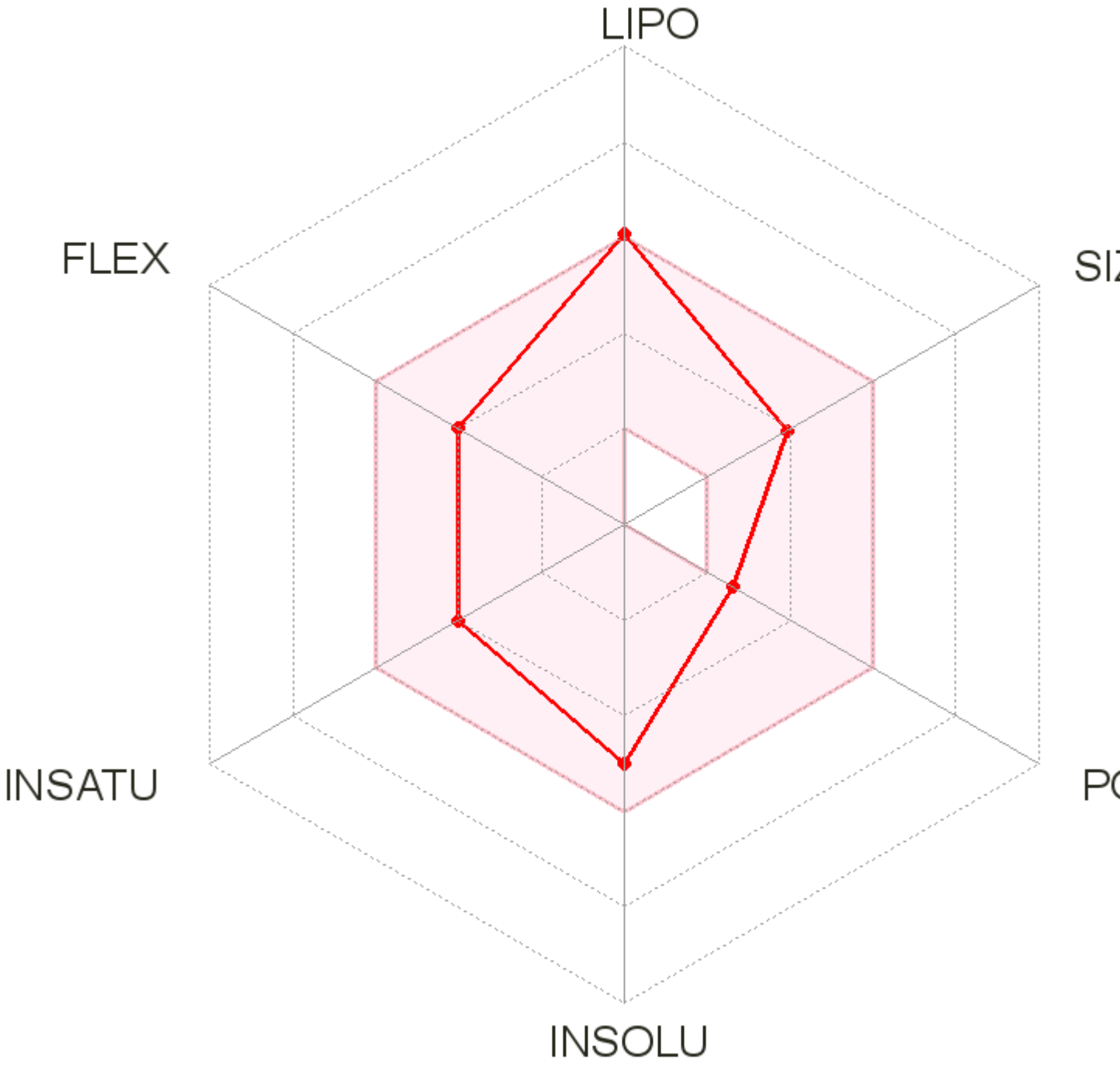
SMILES CN(C[C@H]1CCC[C@H]1CNc1ccnc2c1ccc(c2)Cl)C

Physicochemical Properties

Formula	C18H24ClN3
Molecular weight	317.86 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	10
Fraction Csp3	0.50
Num. rotatable bonds	5
Num. H-bond acceptors	2
Num. H-bond donors	1
Molar Refractivity	95.30
TPSA	28.16 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.53
Log $P_{o/w}$ (XLOGP3)	4.99
Log $P_{o/w}$ (WLOGP)	4.09
Log $P_{o/w}$ (MLOGP)	3.20
Log $P_{o/w}$ (SILICOS-IT)	3.65
Consensus Log $P_{o/w}$	3.89
Water Solubility	
Log *S* (ESOL)	-4.96
Solubility	3.48e-03 mg/ml ; 1.09e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-5.32
Solubility	1.52e-03 mg/ml ; 4.78e-06 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-6.20
Solubility	2.02e-04 mg/ml ; 6.37e-07 mol/l
Class	Poorly soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No

CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-4.70 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	3.06

Molecule 3



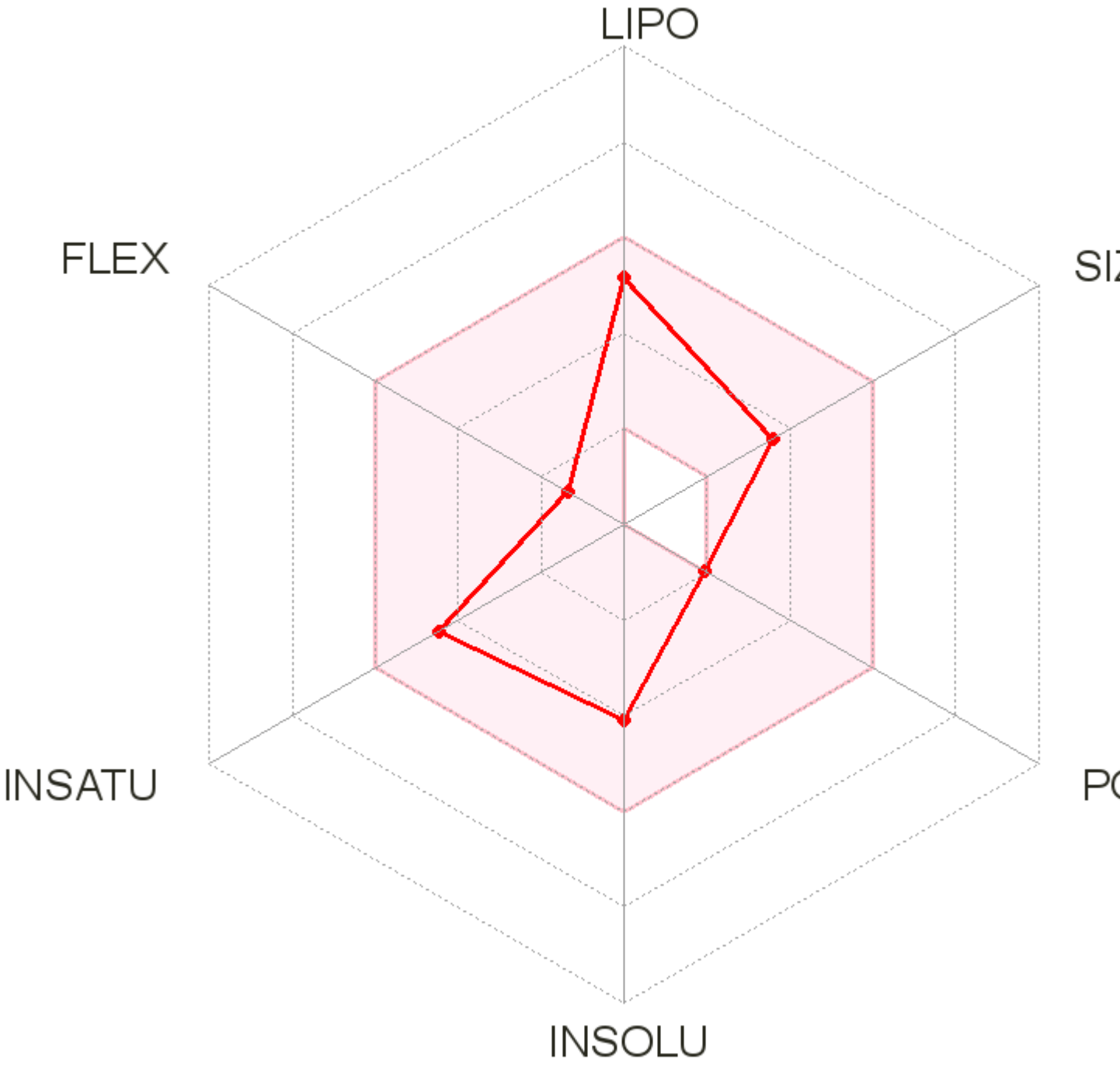
SMILES Clc1ccc2c(c1)nccc2NCCCNC1CCCCC1

Physicochemical Properties

Formula	C18H24ClN3
Molecular weight	317.86 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	10
Fraction Csp3	0.50
Num. rotatable bonds	6
Num. H-bond acceptors	2
Num. H-bond donors	2
Molar Refractivity	95.20
TPSA	36.95 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.72
Log $P_{o/w}$ (XLOGP3)	5.15
Log $P_{o/w}$ (WLOGP)	4.42
Log $P_{o/w}$ (MLOGP)	3.20
Log $P_{o/w}$ (SILICOS-IT)	4.25
Consensus Log $P_{o/w}$	4.15
Water Solubility	
Log *S* (ESOL)	-5.00
Solubility	3.21e-03 mg/ml ; 1.01e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-5.67
Solubility	6.78e-04 mg/ml ; 2.13e-06 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-7.05
Solubility	2.83e-05 mg/ml ; 8.89e-08 mol/l
Class	Poorly soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes

CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.58 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: XLOGP3>5
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.33

Molecule 4



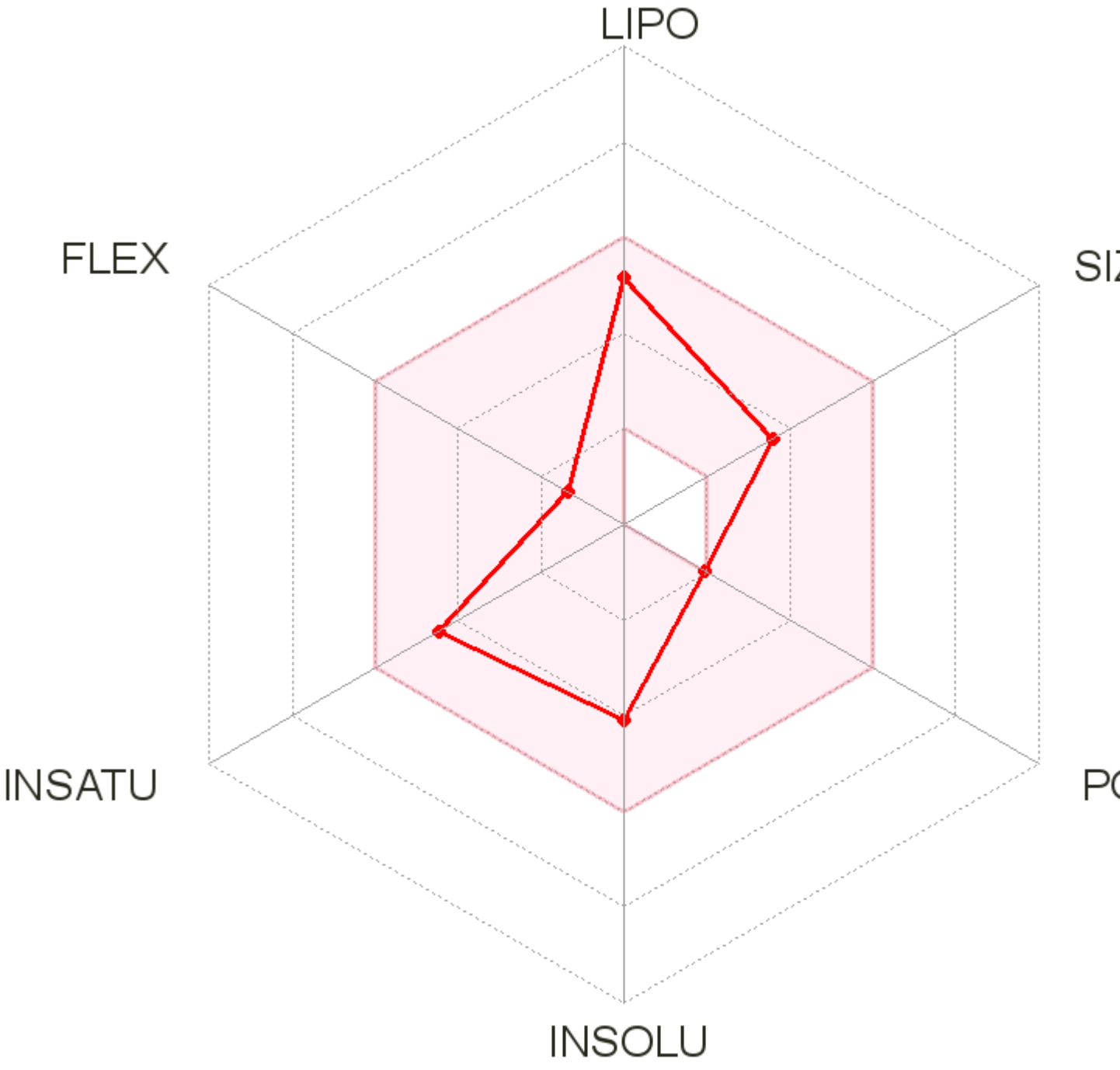
SMILES CN([C@H]1CCCN(C1)c1ccnc2c1ccc(c2)Cl)C

Physicochemical Properties

Formula	C16H20ClN3
Molecular weight	289.80 g/mol
Num. heavy atoms	20
Num. arom. heavy atoms	10
Fraction Csp3	0.44
Num. rotatable bonds	2
Num. H-bond acceptors	2
Num. H-bond donors	0
Molar Refractivity	88.71
TPSA	19.37 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.29
Log $P_{o/w}$ (XLOGP3)	3.53
Log $P_{o/w}$ (WLOGP)	3.04
Log $P_{o/w}$ (MLOGP)	2.73
Log $P_{o/w}$ (SILICOS-IT)	2.83
Consensus Log $P_{o/w}$	3.08
Water Solubility	
Log *S* (ESOL)	-4.10
Solubility	2.31e-02 mg/ml ; 7.97e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-3.62
Solubility	6.94e-02 mg/ml ; 2.39e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-4.92
Solubility	3.52e-03 mg/ml ; 1.22e-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	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.56 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.59

Molecule 5



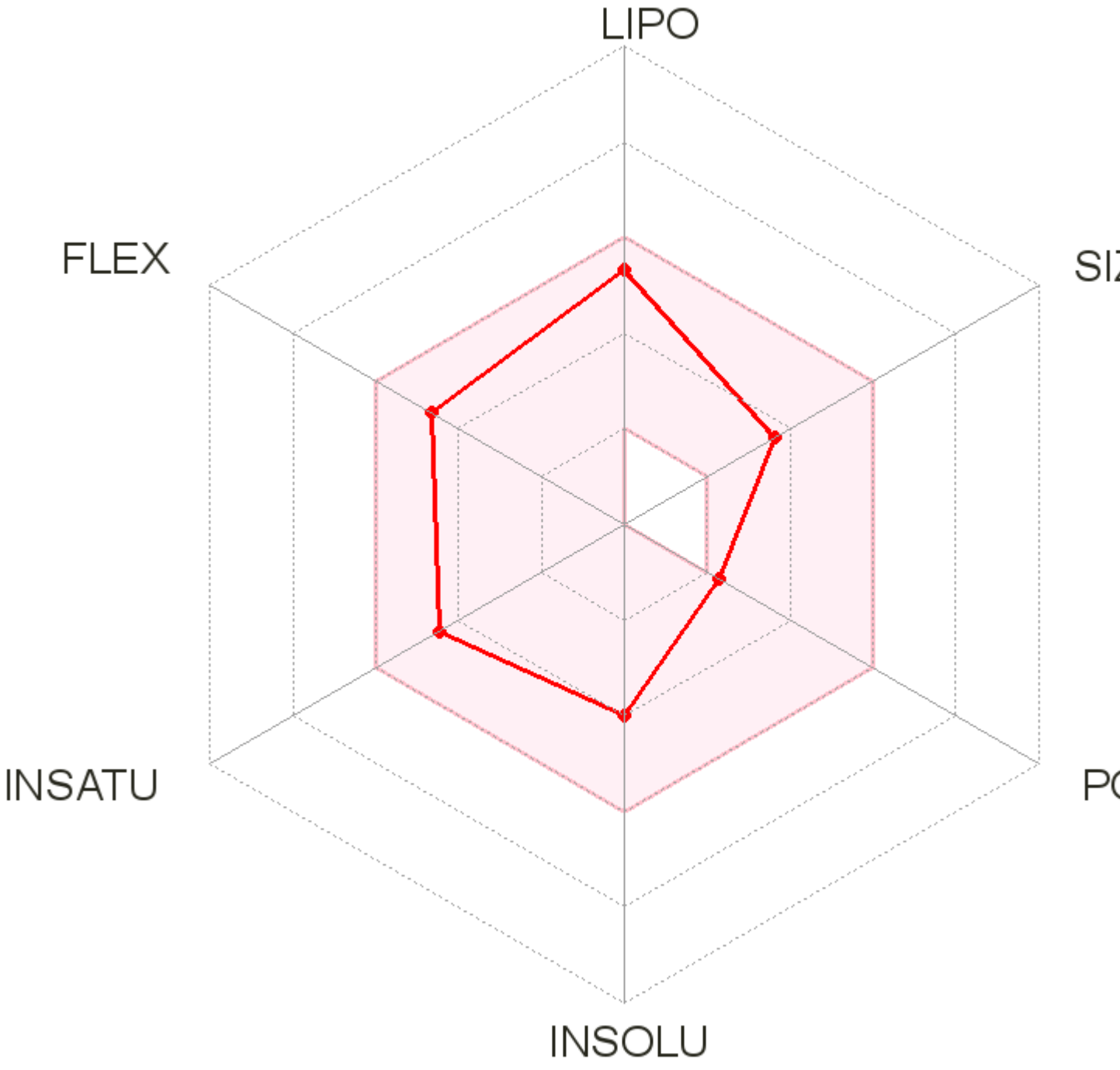
SMILES CN(C1CCCN(C1)c1ccnc2c1ccc(c2)Cl)C

Physicochemical Properties

Formula	C16H20ClN3
Molecular weight	289.80 g/mol
Num. heavy atoms	20
Num. arom. heavy atoms	10
Fraction Csp3	0.44
Num. rotatable bonds	2
Num. H-bond acceptors	2
Num. H-bond donors	0
Molar Refractivity	88.71
TPSA	19.37 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.29
Log $P_{o/w}$ (XLOGP3)	3.53
Log $P_{o/w}$ (WLOGP)	3.04
Log $P_{o/w}$ (MLOGP)	2.73
Log $P_{o/w}$ (SILICOS-IT)	2.83
Consensus Log $P_{o/w}$	3.08
Water Solubility	
Log *S* (ESOL)	-4.10
Solubility	2.31e-02 mg/ml ; 7.97e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-3.62
Solubility	6.94e-02 mg/ml ; 2.39e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-4.92
Solubility	3.52e-03 mg/ml ; 1.22e-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	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.56 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.59

Molecule 6



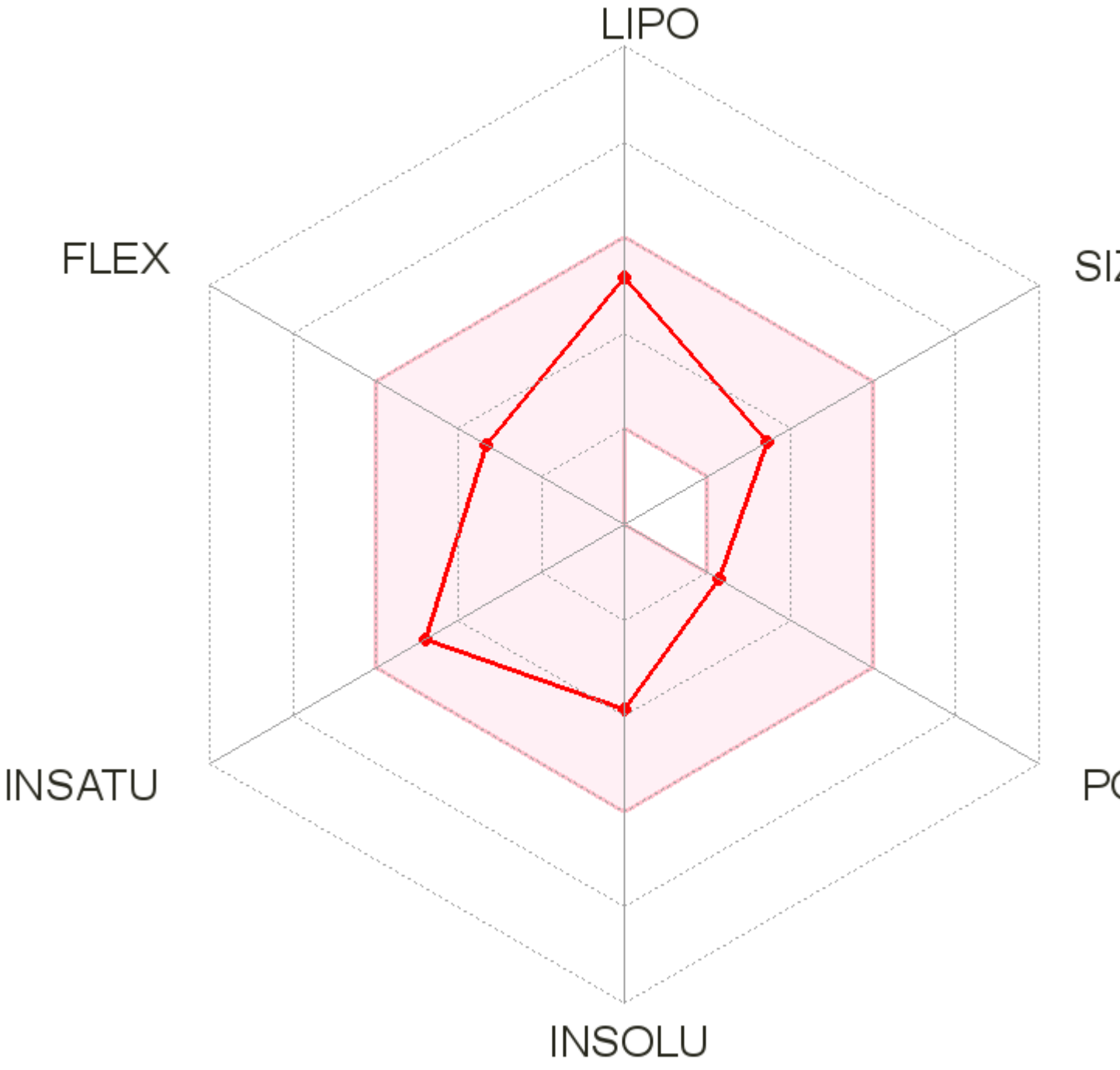
SMILES CCN(CCCNc1ccnc2c1ccc(c2)Cl)CC

Physicochemical Properties

Formula	C16H22ClN3
Molecular weight	291.82 g/mol
Num. heavy atoms	20
Num. arom. heavy atoms	10
Fraction Csp3	0.44
Num. rotatable bonds	7
Num. H-bond acceptors	2
Num. H-bond donors	1
Molar Refractivity	87.80
TPSA	28.16 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.50
Log $P_{o/w}$ (XLOGP3)	3.84
Log $P_{o/w}$ (WLOGP)	3.84
Log $P_{o/w}$ (MLOGP)	2.73
Log $P_{o/w}$ (SILICOS-IT)	3.70
Consensus Log $P_{o/w}$	3.52
Water Solubility	
Log *S* (ESOL)	-3.98
Solubility	3.08e-02 mg/ml ; 1.06e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.13
Solubility	2.18e-02 mg/ml ; 7.46e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-6.50
Solubility	9.31e-05 mg/ml ; 3.19e-07 mol/l
Class	Poorly soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes

CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.35 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.17

Molecule 7



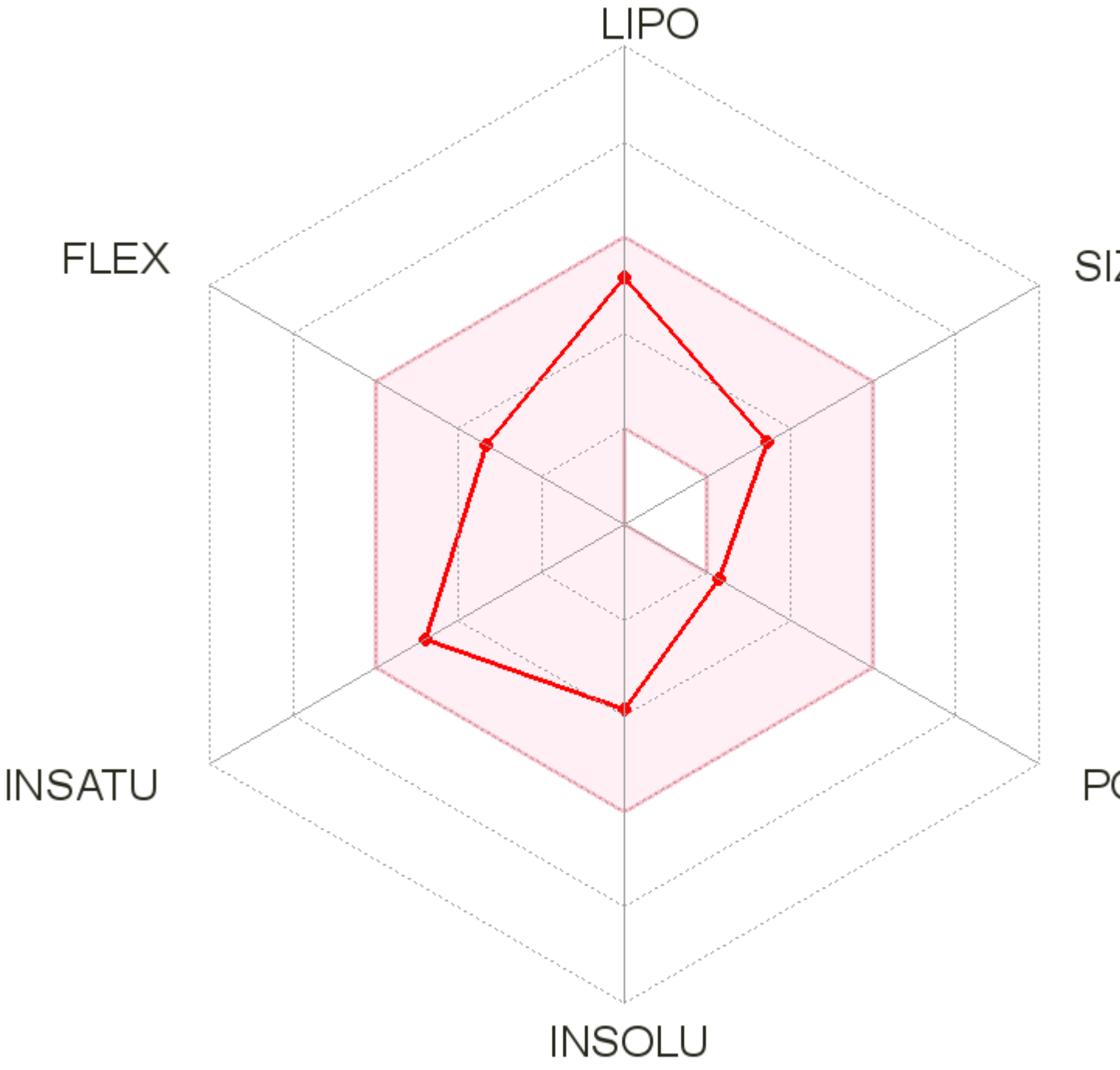
SMILES CN(CCC(Nc1ccnc2c1ccc(c2)Cl)C)C

Physicochemical Properties

Formula	C15H20ClN3
Molecular weight	277.79 g/mol
Num. heavy atoms	19
Num. arom. heavy atoms	10
Fraction Csp3	0.40
Num. rotatable bonds	5
Num. H-bond acceptors	2
Num. H-bond donors	1
Molar Refractivity	82.99
TPSA	28.16 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.09
Log $P_{o/w}$ (XLOGP3)	3.54
Log $P_{o/w}$ (WLOGP)	3.45
Log $P_{o/w}$ (MLOGP)	2.49
Log $P_{o/w}$ (SILICOS-IT)	3.14
Consensus Log $P_{o/w}$	3.14
Water Solubility	
Log *S* (ESOL)	-3.85
Solubility	3.91e-02 mg/ml ; 1.41e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.82
Solubility	4.24e-02 mg/ml ; 1.53e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-5.72
Solubility	5.27e-04 mg/ml ; 1.90e-06 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	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.48 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.49

Molecule 8



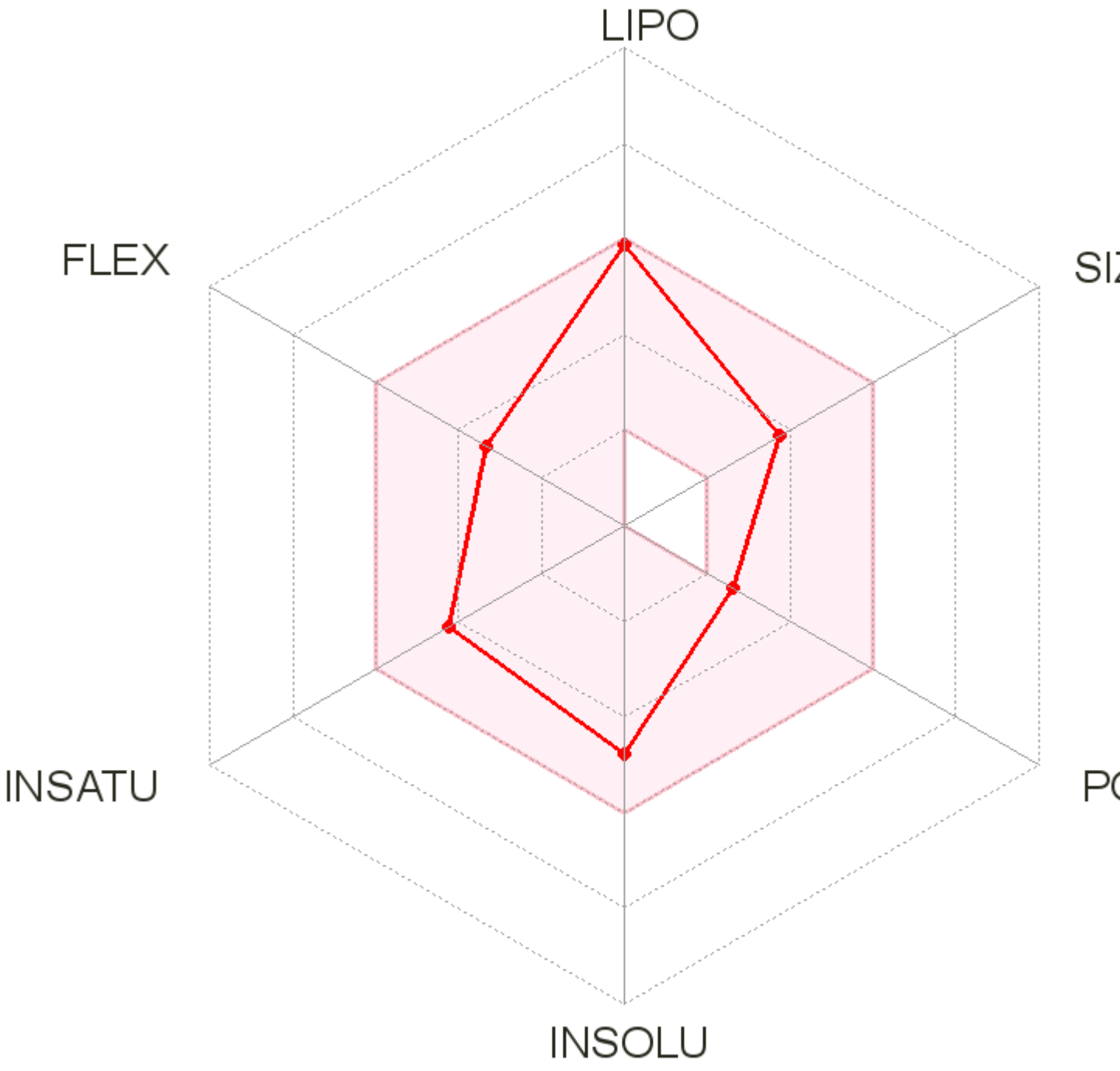
SMILES CN(CCC(Nc1ccnc2c1ccc(c2)Cl)C)C

Physicochemical Properties

Formula	C15H20ClN3
Molecular weight	277.79 g/mol
Num. heavy atoms	19
Num. arom. heavy atoms	10
Fraction Csp3	0.40
Num. rotatable bonds	5
Num. H-bond acceptors	2
Num. H-bond donors	1
Molar Refractivity	82.99
TPSA	28.16 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.09
Log $P_{o/w}$ (XLOGP3)	3.54
Log $P_{o/w}$ (WLOGP)	3.45
Log $P_{o/w}$ (MLOGP)	2.49
Log $P_{o/w}$ (SILICOS-IT)	3.14
Consensus Log $P_{o/w}$	3.14
Water Solubility	
Log *S* (ESOL)	-3.85
Solubility	3.91e-02 mg/ml ; 1.41e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.82
Solubility	4.24e-02 mg/ml ; 1.53e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-5.72
Solubility	5.27e-04 mg/ml ; 1.90e-06 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	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.48 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.49

Molecule 9



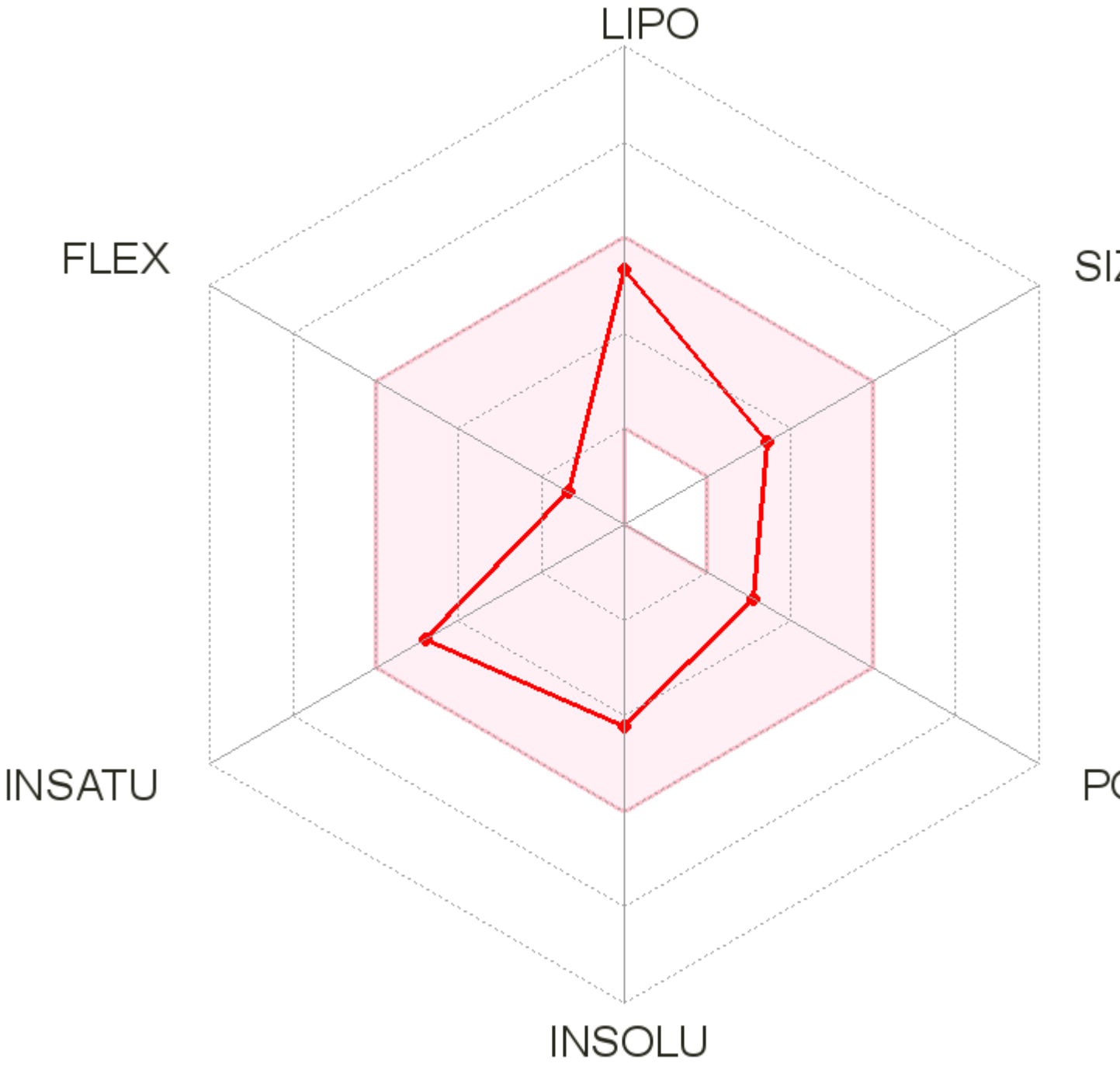
SMILES Clc1ccc2c(c1)nccc2NCCNC1CCCCC1

Physicochemical Properties

Formula	C17H22ClN3
Molecular weight	303.83 g/mol
Num. heavy atoms	21
Num. arom. heavy atoms	10
Fraction Csp3	0.47
Num. rotatable bonds	5
Num. H-bond acceptors	2
Num. H-bond donors	2
Molar Refractivity	90.40
TPSA	36.95 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.47
Log $P_{o/w}$ (XLOGP3)	4.79
Log $P_{o/w}$ (WLOGP)	4.03
Log $P_{o/w}$ (MLOGP)	2.97
Log $P_{o/w}$ (SILICOS-IT)	3.87
Consensus Log $P_{o/w}$	3.83
Water Solubility	
Log *S* (ESOL)	-4.76
Solubility	5.23e-03 mg/ml ; 1.72e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-5.30
Solubility	1.53e-03 mg/ml ; 5.04e-06 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-6.65
Solubility	6.76e-05 mg/ml ; 2.22e-07 mol/l
Class	Poorly soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes

CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.75 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.21

Molecule 10



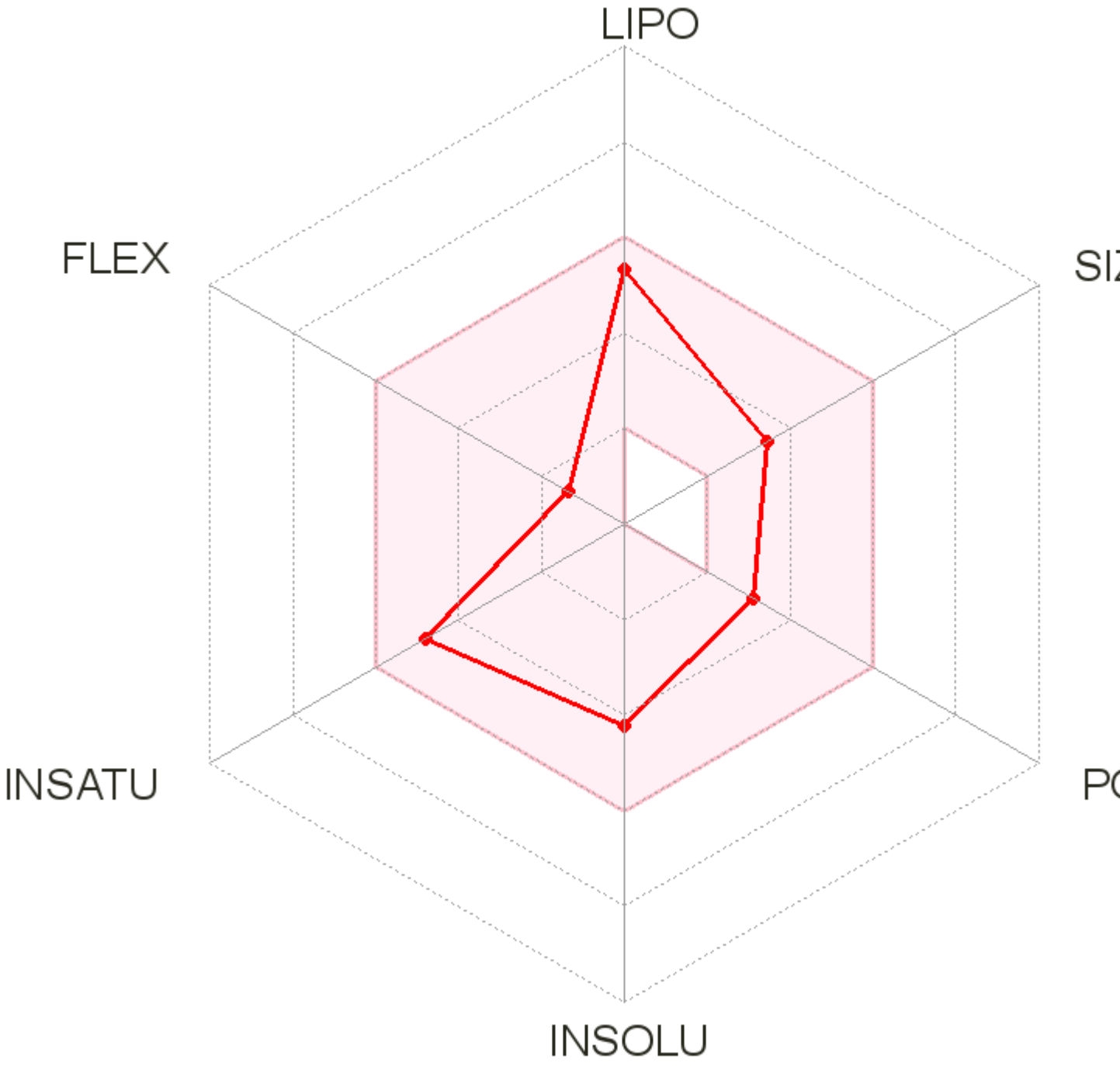
SMILES N[C@H]1CCCC[C@H]1Nc1ccnc2c1ccc(c2)Cl

Physicochemical Properties

Formula	C15H18ClN3
Molecular weight	275.78 g/mol
Num. heavy atoms	19
Num. arom. heavy atoms	10
Fraction Csp3	0.40
Num. rotatable bonds	2
Num. H-bond acceptors	2
Num. H-bond donors	2
Molar Refractivity	80.69
TPSA	50.94 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.69
Log $P_{o/w}$ (XLOGP3)	3.81
Log $P_{o/w}$ (WLOGP)	3.38
Log $P_{o/w}$ (MLOGP)	2.49
Log $P_{o/w}$ (SILICOS-IT)	2.79
Consensus Log $P_{o/w}$	3.03
Water Solubility	
Log *S* (ESOL)	-4.21
Solubility	1.71e-02 mg/ml ; 6.20e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-4.57
Solubility	7.34e-03 mg/ml ; 2.66e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.21
Solubility	1.68e-03 mg/ml ; 6.11e-06 mol/l
Class	Moderately soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	Yes
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes

CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.28 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.71

Molecule 11



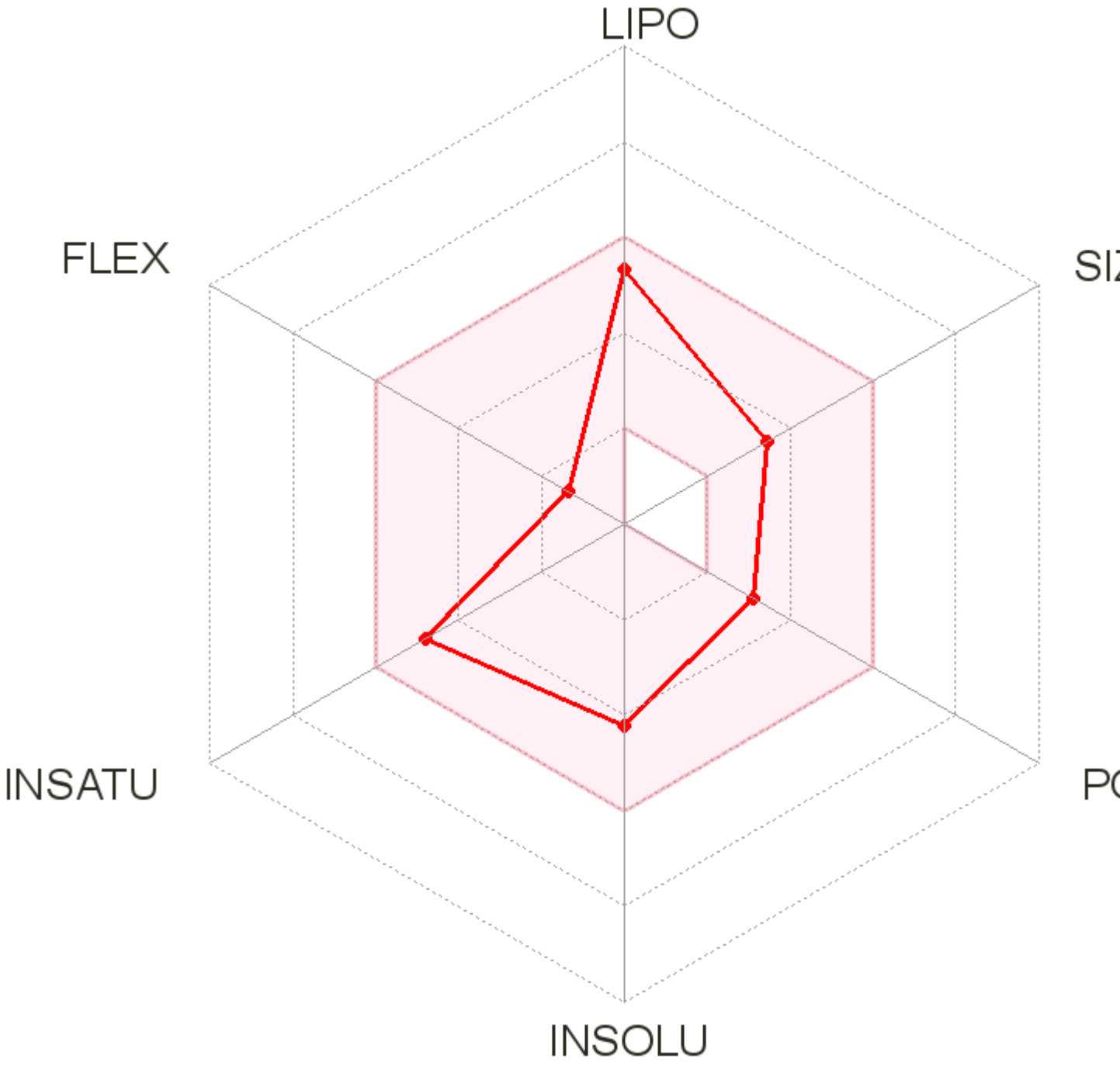
SMILES N[C@@H]1CCCC[C@@H]1Nc1ccnc2c1ccc(c2)Cl

Physicochemical Properties

Formula	C15H18ClN3
Molecular weight	275.78 g/mol
Num. heavy atoms	19
Num. arom. heavy atoms	10
Fraction Csp3	0.40
Num. rotatable bonds	2
Num. H-bond acceptors	2
Num. H-bond donors	2
Molar Refractivity	80.69
TPSA	50.94 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.62
Log $P_{o/w}$ (XLOGP3)	3.81
Log $P_{o/w}$ (WLOGP)	3.38
Log $P_{o/w}$ (MLOGP)	2.49
Log $P_{o/w}$ (SILICOS-IT)	2.79
Consensus Log $P_{o/w}$	3.02
Water Solubility	
Log *S* (ESOL)	-4.21
Solubility	1.71e-02 mg/ml ; 6.20e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-4.57
Solubility	7.34e-03 mg/ml ; 2.66e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-5.21
Solubility	1.68e-03 mg/ml ; 6.11e-06 mol/l
Class	Moderately soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	Yes
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes

CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.28 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.71

Molecule 12



SMILES N[C@H]1CCCC[C@@H]1Nc1ccnc2c1ccc(c2)Cl

Physicochemical Properties

Formula	C15H18ClN3
Molecular weight	275.78 g/mol
Num. heavy atoms	19
Num. arom. heavy atoms	10
Fraction Csp3	0.40
Num. rotatable bonds	2
Num. H-bond acceptors	2
Num. H-bond donors	2
Molar Refractivity	80.69
TPSA	50.94 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.69
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Log $P_{o/w}$ (WLOGP)	3.38
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Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
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Muegge	Yes
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Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	2.71

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