

6-Benzyl-6,7-dihydro-5H-pyrrolo[3,4-B]pyridine
109966-30-5 | DTXSID50364043

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 7.11e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.74e-01

Confidence level: 5.73e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Isouron

Measured: 1.20e-06

Predicted: 1.37e-06

[Image not found](#)

Diphenyl oxide

Measured: 7.39e-04

Predicted: 7.14e-03

[Image not found](#)

Fluridone

Measured: 3.30e-06

Predicted: 8.69e-08

[Image not found](#)

C.I. Disperse Blue 1

Measured: 8.45e-08

Predicted: 1.43e-08