

2-Benzyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine
368441-96-7 | DTXSID50364048

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 6.87e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.24e-01

Confidence level: 7.86e-01

Nearest Neighbors from the Training Set

Image not found

1,3,5-Cycloheptatriene

Measured: 9.69e-11

Predicted: 1.00e-10

Image not found

2-Methyl-p-benzoquinone

Measured: 2.35e-11

Predicted: 2.15e-11