

3-Methyl-1-phenyl-1H-pyrazol-5-amine
1131-18-6 | DTXSID6044517

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.13e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.84e-01

Confidence level: 3.76e-01

Nearest Neighbors from the Training Set

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Ethylenediaminetetraacetic acid

Measured: 1.40e-06

Predicted: 2.81e-12

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2-Phenyl-4,5-dichloro-3-pyridazinone

Measured: 4.50e-07

Predicted: 4.71e-05

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Benzene, 1,4-bis(1-isocyanato-1-methylethyl)-

Measured: 4.50e-07

Predicted: 1.40e-03

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Phenyl glycidyl ether

Measured: 4.36e-04

Predicted: 1.23e-02

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Picloram

Measured: 1.00e-06

Predicted: 1.13e-08