

1,10-Phenanthroline
66-71-7 | DTXSID1025857

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: 4.92e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.97e-01

Confidence level: 4.87e-01

Nearest Neighbors from the Training Set

Image not found

1,2,3,4-Tetrachlorodibenzo-p-dioxin

Measured: 2.00e-06

Predicted: 1.73e-08

Image not found

Isouron

Measured: 1.20e-06

Predicted: 1.37e-06

Image not found

C.I. Disperse Blue 1

Measured: 8.45e-08

Predicted: 1.43e-08

Image not found

Isoamyl ether

Measured: 6.80e-06

Predicted: 1.87

Image not found

Dipropyl phthalate

Measured: 2.48e-03

Predicted: 9.25e-05