

Endothal
145-73-3 | DTXSID7024081

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: 9.06e-10 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.18e-01

Confidence level: 3.69e-01

Nearest Neighbors from the Training Set

Image not found

Oxalic acid

Measured: 1.57e-10

Predicted: 3.33e-04

Image not found

Ethalfuralin

Measured: 1.26e-06

Predicted: 5.55e-05

Image not found

2-Dodecanone

Measured: 6.67e-07

Predicted: 2.01e-02

Image not found

1,2-Benzenedicarbonyl
dichloride

Measured: 6.36e-07

Predicted: 2.89e-03

Image not found

2-Ethoxyethyl acetate

Measured: 5.55e-08

Predicted: 1.46