

Ethanol
64-17-5 | DTXSID9020584

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: 35.3 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.70e-01

Confidence level: 7.50e-01

Nearest Neighbors from the Training Set

Image not found

Carbaryl

Measured: 59.3

Predicted: 1.44e-06

Image not found

Benzene, 1,2-difluoro-

Measured: 21.3

Predicted: 32.2

Image not found

Salicylic acid

Measured: 21.0

Predicted: 2.08e-05

Image not found

Methoxyamine

Measured: 45.4

Predicted: 217

Image not found

Barbituric acid

Measured: 6.70

Predicted: 4.85e-08