

Taurocyamine
543-18-0 | DTXSID10202654

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: 2.58e-09 mmHg

Global applicability domain: Outside

Local applicability domain index: 2.77e-01

Confidence level: 3.51e-01

Nearest Neighbors from the Training Set

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2,2,5,5-Tetramethylhexane

Measured: 9.80e-08

Predicted: 7.94

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2,4,6-Trimethylpyridine

Measured: 3.59e-10

Predicted: 8.58e-01

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4-Oxopentanoic acid

Measured: 1.88e-10

Predicted: 4.67e-03

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1,8-Cineol

Measured: 6.35e-08

Predicted: 1.70

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Benz(a)anthracene

Measured: 1.97e-10

Predicted: 2.14e-08