

Bisphenol A

80-05-7 | DTXSID7020182

Model Performance

Weighted KNN model

5-fold CV (75%)

Training (75%)

Test (25%)

Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 15.1 days

Global applicability domain: Outside

Local applicability domain index: 2.88e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

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9-Ethyl-9H-fluorene

Measured: 29.0

Predicted: N/A

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2-Methylphenanthrene

Measured: 23.0

Predicted: 25.0

[Image not found](#)

5-Methylindan

Measured: 2.00

Predicted: 2.25

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4-Phenyltoluene

Measured: 38.0

Predicted: 25.1

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2-Methylnaphthalene

Measured: 14.0

Predicted: 15.3