

Bisphenol A

80-05-7 | DTXSID7020182

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)

Training (75%)

Test (25%)

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.38

Global applicability domain: Inside

Local applicability domain index: 4.93e-01

Confidence level: 6.05e-01

Nearest Neighbors from the Training Set

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Oxydisulfoton

Measured: 0.0

Predicted: 2.13e-01

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Disulfoton

Measured: 2.34

Predicted: 2.18

[Image not found](#)

Parathion

Measured: 1.99

Predicted: 1.35

[Image not found](#)

O,O-Diethyl dithiophosphate

Measured: 0.7

Predicted: 7.35e-01

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Methyl parathion

Measured: 1.93

Predicted: 1.16