

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: -10.4 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.36e-01

Confidence level: 6.96e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Benzoquinone

Measured: -11.3

Predicted: -11.2

Image not found

2-Methyl-p-benzoquinone

Measured: -10.6

Predicted: -10.7

Image not found

1,3,5-Cycloheptatriene

Measured: -10.0

Predicted: -10.0