

4-Hexylresorcinol
136-77-6 | DTXSID1020699

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.63e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.11e-01

Confidence level: 6.58e-01

Nearest Neighbors from the Training Set

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1,4-Naphthoquinone

Measured: 3.10e-12

Predicted: 3.16e-11

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alpha-Phellandrene

Measured: 3.13e-10

Predicted: 2.83e-10

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2-Methyl-p-benzoquinone

Measured: 2.35e-11

Predicted: 2.15e-11

Image not found

(2E)-2-Hexenal

Measured: 4.40e-11

Predicted: 4.31e-11

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(3Z)-3-Hexenyl acetate

Measured: 7.80e-11

Predicted: 7.52e-11