

beta-Caryophyllene
87-44-5 | DTXSID8024739

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.43e-06 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.86e-01

Confidence level: 7.99e-01

Nearest Neighbors from the Training Set

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Benzene, hexyl-

Measured: 5.56e-06

Predicted: 6.88e-06

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Heptylbenzene

Measured: 2.54e-06

Predicted: 3.24e-06

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tert-Pentylbenzene

Measured: 7.08e-05

Predicted: 3.93e-05

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Cyclopentane, pentyl-

Measured: 8.20e-07

Predicted: 1.76e-06

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p-Menthane

Measured: 2.00e-06

Predicted: 2.12e-06