

Cyclopentane
287-92-3 | DTXSID6024886

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 252 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.59e-01

Confidence level: 8.19e-01

Nearest Neighbors from the Training Set

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Thietane

Measured: 318

Predicted: 31.0

[Image not found](#)

1,5-Hexadiene

Measured: 165

Predicted: 208

[Image not found](#)

1-Butene, 2,3-dimethyl-

Measured: 126

Predicted: 250

[Image not found](#)

Chrysene

Measured: 1170

Predicted: 1.80e-08

[Image not found](#)

Diethyl disulphide

Measured: 96.9

Predicted: 3.38