

9-Propyl-beta-carboline
21373-41-1 | DTXSID90175635

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 50.1

Global applicability domain: Inside

Local applicability domain index: 4.67e-01

Confidence level: 5.49e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Molinate

Measured: 25.7

Predicted: 14.8

[Image not found](#)

Isoamyl ether

Measured: 170

Predicted: 137

[Image not found](#)

Butyl ether

Measured: 72.4

Predicted: 32.3

[Image not found](#)

1-Ethenoxy-2-ethylhexane

Measured: 603

Predicted: 284