

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 128 °C

Global applicability domain: Inside

Local applicability domain index: 6.54e-01

Confidence level: 4.12e-01

Nearest Neighbors from the Training Set

Image not found

Pyrimidine, 4-phenyl-

Measured: 56.0

Predicted: 72.3

Image not found

Imipramine

Measured: 175

Predicted: 145

Image not found

Imipramine hydrochloride

Measured: 174

Predicted: 145

Image not found

Clomipramine

Measured: 190

Predicted: 163

Image not found

Trimipramine

Measured: 45.0

Predicted: 119