

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 331 °C

Global applicability domain: Outside

Local applicability domain index: 4.00e-01

Confidence level: 4.84e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Acibenzolar-S-methyl

Measured: 267

Predicted: 295

[Image not found](#)

2-Methyl-5-nitro-1H-isoindole-
1,3(2H)-dione

Measured: 361

Predicted: 323

[Image not found](#)

4,4'-Methylenebis(N,N-
dimethylaniline)

Measured: 390

Predicted: 349

[Image not found](#)

1,3-Dimethyl-1,3-diphenylurea

Measured: 350

Predicted: 338

[Image not found](#)

3,5-Diphenyl-1,2,4-oxadiazole

Measured: 290

Predicted: 317