

Ethyl 7-ethylcinnoline-3-carboxylate
89770-38-7 | DTXSID00632289

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: 107 °C

Global applicability domain: Inside

Local applicability domain index: 6.15e-01

Confidence level: 5.22e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Pyridazine, 3-(2-methylphenoxy)-

Measured: 78.0

Predicted: 77.2

[Image not found](#)

Pyridaben

Measured: 112

Predicted: 111

[Image not found](#)

Phencarbamide

Measured: 48.5

Predicted: 63.7

[Image not found](#)

Tetrazepam [INN:BAN:DCF]

Measured: 144

Predicted: 137

[Image not found](#)

Diazene, bis(4-ethoxyphenyl)-

Measured: 162

Predicted: 133