

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 96.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.50e-01

Confidence level: 6.86e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ancymidol

Measured: 120

Predicted: 112

[Image not found](#)

Oxycarboxin

Measured: 95.5

Predicted: 175

[Image not found](#)

Diethyl phthalate

Measured: 69.2

Predicted: 102

[Image not found](#)

Carboxin

Measured: 257

Predicted: 210

[Image not found](#)

Dioxacarb

Measured: 39.8

Predicted: 124