

Isopropylpropylamide
80045-52-9 | DTXSID40230046

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.38e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.27e-01

Confidence level: 6.05e-01

Nearest Neighbors from the Training Set

Image not found

Norea

Measured: 6.75e-04

Predicted: 1.66e-03

Image not found

Azacyclotridecan-2-one

Measured: 1.47e-03

Predicted: 1.94e-03