

5-Methylindan
874-35-1 | DTXSID5061245

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 153

Global applicability domain: Inside

Local applicability domain index: 6.33e-01

Confidence level: 7.55e-01

Nearest Neighbors from the Training Set

Image not found

5-Ethylidene-2-norbornene

Measured: 110

Predicted: 134

Image not found

4-Vinylcyclohexene

Measured: 166

Predicted: 158

Image not found

Camphene

Measured: 955

Predicted: 598

Image not found

Dicyclopentadiene

Measured: 219

Predicted: 228

Image not found

Bromobenzene

Measured: 22.9

Predicted: 11.7