

Phenol
108-95-2 | DTXSID5021124

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: 57.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.41e-01

Confidence level: 7.44e-01

Nearest Neighbors from the Training Set

Image not found

Aniline

Measured: 39.8

Predicted: 53.3

Image not found

Phenol

Measured: 26.9

Predicted: 57.3

Image not found

3-Methylaniline

Measured: 33.9

Predicted: 33.3

Image not found

N-Methylaniline

Measured: 191

Predicted: 109

Image not found

Toluene

Measured: 117

Predicted: 87.4