

Anisole
100-66-3 | DTXSID4041608

Model Performance

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: 69.5 L/kg

Global applicability domain: Inside

Local applicability domain index: 7.13e-01

Confidence level: 7.65e-01

Nearest Neighbors from the Training Set

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N-Methylaniline

Measured: 191

Predicted: 109

[Image not found](#)

Acetophenone

Measured: 63.1

Predicted: 67.9

[Image not found](#)

4-Vinylpyridine

Measured: 15.1

Predicted: 43.8

[Image not found](#)

3-Methylaniline

Measured: 33.9

Predicted: 33.3

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4-Methoxyaniline

Measured: 85.1

Predicted: 45.3