

Resorcinol
108-46-3 | DTXSID2021238

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: 28.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.06e-01

Confidence level: 8.56e-01

Nearest Neighbors from the Training Set

Image not found

Benzoic acid

Measured: 31.6

Predicted: 35.5

Image not found

Benzamide

Measured: 28.8

Predicted: 29.7

Image not found

3-Methylaniline

Measured: 33.9

Predicted: 33.3

Image not found

3-Pyridinecarbonitrile

Measured: 36.3

Predicted: 25.0

Image not found

4-Vinylpyridine

Measured: 15.1

Predicted: 43.8