

Endothal
145-73-3 | DTXSID7024081

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: 109 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.33e-01

Confidence level: 6.66e-01

Nearest Neighbors from the Training Set

Image not found

Endothal

Measured: 123

Predicted: 109

Image not found

Cyromazine

Measured: 200

Predicted: 163

Image not found

Dimethyl phthalate

Measured: 39.8

Predicted: 59.9

Image not found

Phthalic acid

Measured: 11.7

Predicted: 21.4

Image not found

Metaldehyde acetaldehyde
tetramer

Measured: 240

Predicted: 148