

Phosphonic acid, bis(1-methylethyl) ester
1809-20-7 | DTXSID7061988

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: 60.2 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.50e-01

Confidence level: 7.22e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Methomyl

Measured: 20.0

Predicted: 39.0

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3-Chlorophenylurea

Measured: 102

Predicted: 57.3

[Image not found](#)

N-(3-chlorophenyl)-N'-methylurea

Measured: 85.1

Predicted: 101

[Image not found](#)

3-Bromophenylurea

Measured: 132

Predicted: 114

[Image not found](#)

Urea, (3-methylphenyl)-

Measured: 36.3

Predicted: 37.2