

meso-Hexestrol
84-16-2 | DTXSID2022381

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: 11800 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.47e-01

Confidence level: 6.60e-01

Nearest Neighbors from the Training Set

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Diethylstilbestrol

Measured: 13800

Predicted: 6630

[Image not found](#)

Bifenox

Measured: 10000

Predicted: 3180

[Image not found](#)

Butralin

Measured: 9550

Predicted: 7850

[Image not found](#)

Niclosamide

Measured: 2240

Predicted: 4670

[Image not found](#)

Methoxychlor

Measured: 79400

Predicted: 5520