

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 157 °C

Global applicability domain: Inside

Local applicability domain index: 8.47e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

[Image not found](#)

meso-Hexestrol

Measured: 187

Predicted: 157

[Image not found](#)

Bisphenol B

Measured: 121

Predicted: 140

[Image not found](#)

phenol, 4,4'-butylidenebis-

Measured: 137

Predicted: 142

[Image not found](#)

Bisphenol A

Measured: 153

Predicted: 144

[Image not found](#)

3,3'-Dimethylbisphenol A

Measured: 139

Predicted: 157