

3,6-Diacetylmorphine
561-27-3 | DTXSID6046761

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 10.7

Global applicability domain: Inside

Local applicability domain index: 9.60e-01

Confidence level: 4.09e-01

Nearest Neighbors from the Training Set

Image not found

Endosulfan I

Measured: 8.64

Predicted: 10.7

Image not found

1,2,3,4,7,8,9-

Heptachlorodibenzofuran

Measured: 11.4

Predicted: 10.9

Image not found

1,2,3,4,6,7,8-

Heptachlorodibenzo[b,d]furan

Measured: 11.2

Predicted: 10.9

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2,2',3,4,4'-Pentabromodiphenyl
ether (BDE 85)

Measured: 11.7

Predicted: 11.5

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1,2,3,4,6,7,8-

Heptachlorodibenzodioxin

Measured: 11.4

Predicted: 10.4