

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 63400 L/kg

Global applicability domain: Outside

Local applicability domain index: 1.54e-01

Confidence level: 4.71e-01

Nearest Neighbors from the Training Set

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C.I. Vat Yellow 4

Measured: 19100

Predicted: 50300

Image not found

Rotenone

Measured: 10000

Predicted: 48700

Image not found

Dieldrin

Measured: 12000

Predicted: 16200

Image not found

Endrin

Measured: 12000

Predicted: 16200

Image not found

Dibenzo[a,i]pyrene

Measured: 513000

Predicted: 203000

Image not found

Indeno(1,2,3-cd)pyrene

Measured: 1580000

Predicted: 233000