

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 179 °C

Global applicability domain: Inside

Local applicability domain index: 4.62e-01

Confidence level: 5.00e-01

Nearest Neighbors from the Training Set

[Image not found](#)

3,6-Diacetylmorphine

Measured: 173

Predicted: 179

[Image not found](#)

Mepixanox

Measured: 160

Predicted: 150

[Image not found](#)

Thebaine

Measured: 193

Predicted: 169

[Image not found](#)

Oxycodone

Measured: 219

Predicted: 207