

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.56e-10 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 9.33e-02

Confidence level: 8.81e-01

Nearest Neighbors from the Training Set

Image not found

alpha-Humulene

Measured: 2.90e-10

Predicted: 2.87e-10

Image not found

Ocimene (E)

Measured: 2.52e-10

Predicted: 2.40e-10

Image not found

beta-Ocimene

Measured: 2.52e-10

Predicted: 2.40e-10

Image not found

Myrcene

Measured: 2.15e-10

Predicted: 2.05e-10

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Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

Measured: 4.80e-11

Predicted: 4.73e-11