

Deacetylmoxisylyte
35231-36-8 | DTXSID10188722

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: 63.7 °C

Global applicability domain: Inside

Local applicability domain index: 4.95e-01

Confidence level: 5.82e-01

Nearest Neighbors from the Training Set

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Methylephedrine

Measured: 87.5

Predicted: 90.6

[Image not found](#)

Glycine, N-phenyl-, ethyl ester

Measured: 58.0

Predicted: 41.6

[Image not found](#)

4-Piperidinol, 1-methyl-

Measured: 29.0

Predicted: 41.0

[Image not found](#)

Hordeine

Measured: 118

Predicted: 90.8

[Image not found](#)

Methyl 2-(methylamino)benzoate

Measured: 19.0

Predicted: 23.7