

Deacetylmoxisylyte
35231-36-8 | DTXSID10188722

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 277 °C

Global applicability domain: Inside

Local applicability domain index: 3.03e-01

Confidence level: 6.74e-01

Nearest Neighbors from the Training Set

Image not found

3-Diethylaminophenol

Measured: 276

Predicted: 270

Image not found

Ethanol, 2-(ethylphenylamino)-

Measured: 268

Predicted: 270

Image not found

2-(2-Nitrophenyl)ethanol

Measured: 267

Predicted: 269

Image not found

Lupinine

Measured: 270

Predicted: 259

Image not found

4-Octylaniline

Measured: 310

Predicted: 287