

Arginine
7200-25-1 | DTXSID8022618

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.61e-01 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.49e-01

Confidence level: 5.54e-01

Nearest Neighbors from the Training Set

Image not found

Arginine

Measured: 1.04

Predicted: 7.61e-01

Image not found

Azidamfenicol [INN:BAN:DCF]

Measured: 6.77e-02

Predicted: 4.38e-02

Image not found

Cyanoguanidine

Measured: 4.91e-01

Predicted: 2.09e-01