

Carboxymethyl cellulose

9000-11-7 | DTXSID7040441

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)

Training (75%)

Test (25%)

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 5.09e-01

Global applicability domain: Inside

Local applicability domain index: 1.99e-01

Confidence level: 8.71e-01

Nearest Neighbors from the Training Set

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Tris(2-hydroxyethyl)
isocyanurate

Measured: 0.2

Predicted: 2.08e-01

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2-Amino-5-
methylbenzenesulfonic acid

Measured: 0.6

Predicted: 7.98e-01

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7-Amino-4-
hydroxynaphthalene-2-
sulfonic acid

Measured: 0.38

Predicted: 6.78e-01

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6-Amino-4-
hydroxynaphthalene-2-
sulfonic acid

Measured: 0.61

Predicted: 6.78e-01

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2-Amino-1-
naphthalenesulfonic acid

Measured: 0.78

Predicted: 8.06e-01