

Methyl beta-alanate
4138-35-6 | DTXSID50194322

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 8.53e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.16e-01

Confidence level: 5.77e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Urethane

Measured: 2.62e-01

Predicted: 3.29e-01

[Image not found](#)

Tetraethyl orthosilicate

Measured: 7.00e-01

Predicted: 2.76

[Image not found](#)

Chloroacetyl chloride

Measured: 3.78e-02

Predicted: 33.9

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Ethane-1,2-dithiol

Measured: 3.91e-03

Predicted: 3.98