

PUBCHEM_54605649

40730-78-7 | DTXSID90714109

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: 8.11e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.04e-01

Confidence level: 3.10e-01

Nearest Neighbors from the Training Set

No Similar Structures Found.