

Predicted Thermal conductivity at 25 °C for [110-91-8](#) from Consensus method

Prediction results

Endpoint	Experimental value	Predicted value
Thermal conductivity at 25 °C mW/mK	N/A	173.16

Individual Predictions		Test chemical
Method	Predicted value mW/mK	
Hierarchical clustering	178.78	
Single model	167.55	
Group contribution	N/A	
Nearest neighbor	N/A	

Predictions for the test chemical and for the most similar chemicals in the [external test set](#)

Note: No chemicals in the test set exceed a minimum similarity coefficient of 0.5 for comparison purposes

Predictions for the test chemical and for the most similar chemicals in the [training set](#)

If the predicted value matches the experimental values for similar chemicals in the training set (and the similar chemicals were predicted well), one has greater confidence in the predicted value.

□	Chemicals	MAE*
	Entire set	6.18
	Similarity coefficient ≥ 0.5	8.53

*Mean absolute error in mW/mK

CAS	Structure	Similarity Coefficient	Experimental value mW/mK	Predicted value mW/mK
110-91-8			N/A	173.16

109-89-7		0.95	175.40	158.91
103-69-5		0.55	150.30	150.86