

## Predicted Thermal conductivity at 25 °C for 69-72-7 from Consensus method

Prediction results

Endpoint	Experimental value	Predicted value <sup>b</sup>
Thermal conductivity at 25 °C mW/mK	N/A	N/A

<sup>b</sup>The consensus prediction for this chemical is considered unreliable since only one prediction can only be made

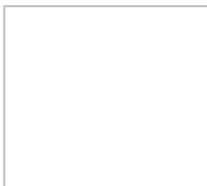
Individual Predictions		Test chemical
<b>Method</b>	<b>Predicted value mW/mK</b>	
Hierarchical clustering	N/A	
Single model	N/A	
Group contribution	N/A	
Nearest neighbor	146.37	

## Predictions for the test chemical and for the most similar chemicals in the external test set

If *similar* test set chemicals were predicted well relative to the entire test set, one has greater confidence in the predicted value.

Chemicals	MAE*
Entire set	7.05
Similarity coefficient $\geq 0.5$	0.44

\*Mean absolute error in mW/mK

CAS	Structure	Similarity Coefficient	Experimental value mW/mK	Predicted value mW/mK
69-72-7 (test chemical)			N/A	N/A
108-39-4		0.68	148.67	149.10

## 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 $\geq 0.5$	4.54

\*Mean absolute error in mW/mK

CAS	Structure	Similarity Coefficient	Experimental value mW/mK	Predicted value mW/mK
69-72-7 (test chemical)			N/A	N/A
106-44-5		0.73	144.40	147.91
95-48-7		0.71	153.60	148.14
95-57-8		0.70	141.10	143.18
108-95-2		0.61	159.53	150.62
100-51-6		0.58	159.43	156.39

89-83-8		0.56	131.00	136.31
93-58-3		0.52	146.90	143.43