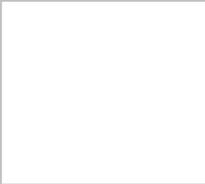


## Predicted Vapor pressure at 25 °C for 1897-45-6 from Consensus method

Prediction results

Endpoint	Experimental value (CAS= 1897-45-6) Source: EPI Suite v 4.00	Predicted value <sup>a</sup>
Vapor pressure at 25 °C Log10(mmHg)	-6.24	-3.66
Vapor pressure at 25 °C mmHg	5.70E-07	2.21E-04

<sup>a</sup>Note: the test chemical was present in the training set. The prediction *does not* represent an external prediction.

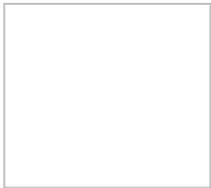
Individual Predictions		Test chemical
<b>Method</b>	<b>Predicted value Log10(mmHg)</b>	
Hierarchical clustering	-5.21	
Group contribution	-5.43	
Nearest neighbor	-0.32	

## 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	0.47
Similarity coefficient $\geq 0.5$	0.01

\*Mean absolute error in Log10(mmHg)

CAS	Structure	Similarity Coefficient	Experimental value Log10(mmHg)	Predicted value Log10(mmHg)
1897-45-6 (test chemical)			-6.24	-3.66
100-54-9		0.71	-0.53	-0.54

## 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	0.40
Similarity coefficient $\geq 0.5$	0.83

\*Mean absolute error in Log10(mmHg)

CAS	Structure	Similarity Coefficient	Experimental value Log10(mmHg)	Predicted value Log10(mmHg)
1897-45-6 (test chemical)			-6.24	-3.66
104-85-8		0.74	-0.50	-1.04
529-19-1		0.74	-0.35	-1.00
100-47-0		0.71	-0.12	-0.82
1689-99-2		0.63	-5.32	-6.63
74738-17-3		0.53	-7.08	-6.13

