

Predicted Surface tension at 25 °C for 1897-45-6 from Consensus method

Prediction results

| Endpoint | Experimental value | Predicted value ^b |
|---------------------------------|--------------------|------------------------------|
| Surface tension at 25 °C dyn/cm | N/A | N/A |

^bThe consensus prediction for this chemical is considered unreliable since only one prediction can only be made

| Individual Predictions | | Test chemical |
|-------------------------|------------------------|---|
| Method | Predicted value dyn/cm |  |
| Hierarchical clustering | N/A | |
| Group contribution | N/A | |
| Nearest neighbor | 36.34 | |

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 | 1.16 |
| Similarity coefficient ≥ 0.5 | 0.80 |

*Mean absolute error in dyn/cm

| CAS | Structure | Similarity Coefficient | Experimental value dyn/cm | Predicted value dyn/cm |
|------------------------------|-----------|------------------------|---------------------------|------------------------|
| 1897-45-6 (test chemical) | | | N/A | N/A |

| | | | | |
|------------|--|------|-------|-------|
| | | | | |
| 541-73-1 | | 0.58 | 35.43 | 34.55 |
| 61142-85-6 | | 0.53 | 36.32 | 37.59 |
| 529-19-1 | | 0.53 | 37.28 | 36.85 |
| 4939-73-5 | | 0.52 | 37.04 | 37.67 |