

1,4-Diazabicyclo[2.2.2]octane  
280-57-9 | DTXSID0022016

### 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
0.81	0.55	0.81	0.54	0.71	0.61

## Model Results

**Predicted value:** 82.2 L/kg

**Global applicability domain:** Outside

**Local applicability domain index:** 2.03e-01

**Confidence level:** 5.67e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Dazomet

**Measured:** 10.0

**Predicted:** 16.0

[Image not found](#)

Thiram

**Measured:** 676

**Predicted:** 493

[Image not found](#)

Nicotine

**Measured:** 102

**Predicted:** 122

[Image not found](#)

Methapyrilene

**Measured:** 741

**Predicted:** 682

[Image not found](#)

N,N-Dimethylaniline

**Measured:** 182

**Predicted:** 130