# Yasuda-Shedlovsky Result

| | | | |
|---|---|---|---|
| Sample name: | **CS000055** | Experiment start time: | **28/07/2011 14:32:28** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11G-28009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1107\11G-28009_CS000055_pH-metric psKa.t3r** | | |

## Yasuda-Shedlovsky result

| Extrapolation type | pKa 0% | SD | Intercept | Slope | $R^2$ | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|
| Yasuda-Shedlovsky | 6.67 | ±0.01 | 4.59 | 298.5450 | 1.0000 | 0.175 M | 26.4°C |

## Component assay results

| Titration | Methanol weight% | Direction | Result type | Dielectric constant | [H2O] | Ionic strength | Temperature | | psKa 1 |
|---|---|---|---|---|---|---|---|---|---|
| 11G-28009 Points 97 to 142 | 35.17 % | Up | pH-metric | 62.4 | 32.7 M | 0.184 M | 27.4°C | ☑ | 7.86 |
| 11G-28009 Points 51 to 96 | 48.66 % | Up | pH-metric | 56.4 | 25.1 M | 0.178 M | 26.9°C | ☑ | 8.49 |
| 11G-28009 Points 3 to 50 | 65.65 % | Up | pH-metric | 48.9 | 16.2 M | 0.164 M | 25.1°C | ☑ | 9.48 |

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000055** | Experiment start time: | **28/07/2011 14:32:28** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11G-28009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1107\11G-28009_CS000055_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 1 of 3 11G-28009 Points 3 to 50

## Sample

| | |
|---|---|
| CS000055 concentration factor | 1.000 |
| Base pKa 1 | 9.48 |

## Sample graphs

## Other graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000055** | Experiment start time: | **28/07/2011 14:32:28** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11G-28009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1107\11G-28009_CS000055_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 2 of 3 11G-28009 Points 51 to 96

## Sample

| | |
|---|---|
| CS000055 concentration factor | 1.000 |
| Base pKa 1 | 8.49 |

## Sample graphs

## Other graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000055** | Experiment start time: | **28/07/2011 14:32:28** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11G-28009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1107\11G-28009_CS000055_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 3 of 3 11G-28009 Points 97 to 142

## Sample

- CS000055 concentration factor 0.873
- Base pKa 1 7.86

## Sample graphs

## Other graphs

## Assay Model

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| Sample name | CS000055 | | |
| Sample by | Weight | | |
| Sample weight | 0.001080 g | | |
| Formula weight | 303.32 g/mol | | |
| Solubility | Unknown | | |
| Molecular weight | 303.32 | | |
| Individual pKa ionic environments | No | | |
| Number of pKas | 1 | | |
| Sample is a | Base | | |
| pKa 1 | 4.00 | | |
| logp (XH +) | -10.00 | | |
| logP (neutral X) | -10.00 | | |