# Yasuda-Shedlovsky Result

| | | | |
|---|---|---|---|
| Sample name: | **CS000100** | Experiment start time: | **31/07/2011 14:19:21** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11G-31007** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r** | | |

## Yasuda-Shedlovsky result

| Extrapolation type | pKa 0% | SD | Intercept | Slope | R² | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|
| Yasuda-Shedlovsky | 4.80 | ±0.02 | 9.89 | -261.5667 | 0.9996 | 0.174 M | 26.0°C |
| Yasuda-Shedlovsky | 9.97 | ±0.23 | 13.66 | -152.2735 | 0.8459 | 0.174 M | 26.0°C |

## Component assay results

| Titration | Methanol weight% | Direction | Result type | Dielectric constant | [H2O] | Ionic strength | Temperature | | psKa 1 | | I |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 11G-31007 Points 105 to 153 | 27.33 % | Up | pH-metric | 66.1 | 37.4 M | 0.182 M | 26.6°C | ☑ | 4.36 | ☑ | 8 |
| 11G-31007 Points 53 to 104 | 37.04 % | Up | pH-metric | 62.0 | 31.7 M | 0.175 M | 26.0°C | ☑ | 4.18 | ☑ | 6 |
| 11G-31007 Points 3 to 52 | 48.19 % | Up | pH-metric | 57.1 | 25.4 M | 0.164 M | 25.3°C | ☑ | 3.90 | ☑ | 6 |

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000100** | Experiment start time: | **31/07/2011 14:19:21** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11G-31007** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 1 of 3 11G-31007 Points 3 to 52

## Sample

| | |
|---|---|
| CS000100 concentration factor | 0.882 |
| Base pKa 1 | 3.90 |
| Base pKa 2 | 9.62 |

## Sample graphs

## Other graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000100** | Experiment start time: | **31/07/2011 14:19:21** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11G-31007** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 2 of 3 11G-31007 Points 53 to 104

## Sample

| | |
|---|---|
| CS000100 concentration factor | 0.884 |
| Base pKa 1 | 4.18 |
| Base pKa 2 | 9.61 |

## Sample graphs

## Other graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000100** | Experiment start time: | **31/07/2011 14:19:21** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11G-31007** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 3 of 3 11G-31007 Points 105 to 153

## Sample

| | |
|---|---|
| CS000100 concentration factor | 0.902 |
| Base pKa 1 | 4.36 |
| Base pKa 2 | 9.83 |

## Sample graphs

## Other graphs

## Assay Model

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| Sample name | CS000100 | | |
| Sample by | Weight | 31/07/2011 10:48:23 | E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r |
| Sample weight | 0.001100 g | | |
| Formula weight | 473.30 g/mol | | |
| Solubility | Unknown | 31/07/2011 10:48:23 | E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r |
| Molecular weight | 473.30 | | |
| Individual pKa ionic environments | No | | |
| Number of pKas | 2 | 31/07/2011 10:48:23 | E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r |
| Sample is a | Base | 31/07/2011 10:48:23 | E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r |
| pKa 1 | 4.00 | 31/07/2011 10:48:23 | E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r |

| | | | |
|---|---|---|---|
| Sample name: | **CS000100** | Experiment start time: | **31/07/2011 14:19:21** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11G-31007** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r** | | |

## Assay Model (continued)

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| pKa 2 | 8.00 | 31/07/2011 10:48:23 | E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r |
| logP (XH2 2+) | -10.00 | 31/07/2011 10:48:23 | E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r |
| logp (XH +) | -10.00 | 31/07/2011 10:48:23 | E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r |
| logP (neutral X) | -10.00 | 31/07/2011 10:48:23 | E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r |