# Yasuda-Shedlovsky Result

| | | | |
|---|---|---|---|
| Sample name: | **cs000115** | Experiment start time: | **22/08/2011 17:12:22** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-22013** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-22013_cs000115_pH-metric psKa.t3r** | | |

## Yasuda-Shedlovsky result

| Extrapolation type | pKa 0% | SD | Intercept | Slope | R² | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|
| Yasuda-Shedlovsky | 2.24 | ±0.04 | 5.57 | -123.4060 | 0.9914 | 0.176 M | 26.2°C |
| Yasuda-Shedlovsky | 10.88 | ±0.03 | 13.15 | -41.7175 | 0.9482 | 0.176 M | 26.2°C |

## Component assay results

| Titration | Methanol weight% | Direction | Result type | Dielectric constant | [H2O] | Ionic strength | Temperature | | psKa 1 | | sK |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 11H-22013 Points 68 to 107 | 26.50 % | Up | pH-metric | 66.3 | 37.9 M | 0.185 M | 27.1°C | ☑ | 2.14 | ☑ | ).9 |
| 11H-22013 Points 34 to 67 | 36.27 % | Up | pH-metric | 62.2 | 32.1 M | 0.178 M | 26.5°C | ☑ | 2.06 | ☑ | ).9 |
| 11H-22013 Points 3 to 33 | 47.68 % | Up | pH-metric | 57.4 | 25.7 M | 0.166 M | 25.1°C | ☑ | 2.01 | ☑ | ..( |

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **cs000115** | Experiment start time: | **22/08/2011 17:12:22** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-22013** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-22013_cs000115_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 1 of 3 11H-22013 Points 3 to 33

## Sample

| | |
|---|---|
| cs000115 concentration factor | 1.374 |
| Base pKa 1 | 2.01 |
| Base pKa 2 | 11.02 |

## Sample graphs

## Other graphs

| | | | |
|---|---|---|---|
| Sample name: | **cs000115** | Experiment start time: | **22/08/2011 17:12:22** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-22013** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-22013_cs000115_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 2 of 3 11H-22013 Points 34 to 67

## Sample

| | |
|---|---|
| cs000115 concentration factor | 1.413 |
| Base pKa 1 | 2.06 |
| Base pKa 2 | 10.96 |

## Sample graphs

## Other graphs

| | | | |
|---|---|---|---|
| Sample name: | **cs000115** | Experiment start time: | **22/08/2011 17:12:22** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-22013** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-22013_cs000115_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 3 of 3 11H-22013 Points 68 to 107

## Sample

| | |
|---|---|
| cs000115 concentration factor | 1.171 |
| Base pKa 1 | 2.14 |
| Base pKa 2 | 10.95 |

## Sample graphs

## Other graphs

## Assay Model

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| Sample name | cs000115 | | |
| Sample by | Weight | 22/08/2011 13:07:31 | E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r |
| Sample weight | 0.000870 g | | |
| Formula weight | 297.32 g/mol | | |
| Solubility | Unknown | 22/08/2011 13:07:31 | E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r |
| Molecular weight | 297.32 | | |
| Individual pKa ionic environments | No | | |
| Number of pKas | 2 | | |
| Sample is a | Base | 22/08/2011 13:07:31 | E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r |
| pKa 1 | 3.20 | | |
| pKa 2 | 10.20 | | |
| logP (XH2 2+) | -10.00 | 22/08/2011 13:07:31 | E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r |

| | | | |
|---|---|---|---|
| Sample name: | **cs000115** | Experiment start time: | **22/08/2011 17:12:22** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-22013** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-22013_cs000115_pH-metric psKa.t3r** | | |

## Assay Model (continued)

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| logp (XH +) | -10.00 | | |
| logP (neutral X) | -10.00 | | |