# Yasuda-Shedlovsky Result

| | | | |
|---|---|---|---|
| Sample name: | **CS000100** | Experiment start time: | **12/08/2011 10:59:15** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-12005** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-12005_CS000100_pH-metric psKa.t3r** | | |

## Yasuda-Shedlovsky result

| Extrapolation type | pKa 0% | SD | Intercept | Slope | R² | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|
| Yasuda-Shedlovsky | 4.48 | ±0.22 | 31.67 | -1982.3011 | 0.8697 | 0.190 M | 26.8°C |
| Yasuda-Shedlovsky | 9.29 | ±0.36 | -37.20 | 3758.0078 | 0.8968 | 0.190 M | 26.8°C |

## Component assay results

| Titration | DMSO weight% | Direction | Result type | Dielectric constant | [H2O] | Ionic strength | Temperature | | psKa 1 | | sK |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 11H-12005 Points 85 to 129 | 21.95 % | Up | pH-metric | 76.6 | 44.0 M | 0.196 M | 27.3°C | ✓ | 4.14 | ✓ | 0.1 |
| 11H-12005 Points 44 to 84 | 29.59 % | Up | pH-metric | 76.2 | 40.0 M | 0.191 M | 27.2°C | ✓ | 4.11 | ✓ | 0.6 |
| 11H-12005 Points 3 to 43 | 38.42 % | Up | pH-metric | 75.9 | 35.3 M | 0.182 M | 25.9°C | ✓ | 3.98 | ✓ | 0.7 |

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000100** | Experiment start time: | **12/08/2011 10:59:15** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-12005** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-12005_CS000100_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 1 of 3 11H-12005 Points 3 to 43 Quality: Good

## Sample

| | |
|---|---|
| CS000100 concentration factor | 0.467 |
| Base pKa 1 | 3.98 |
| Base pKa 2 | 10.70 |

## Sample graphs

## Other graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000100** | Experiment start time: | **12/08/2011 10:59:15** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-12005** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-12005_CS000100_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 2 of 3 11H-12005 Points 44 to 84 Quality: Good

## Sample

| | |
|---|---|
| CS000100 concentration factor | 0.496 |
| Base pKa 1 | 4.11 |
| Base pKa 2 | 10.60 |

## Sample graphs

## Other graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000100** | Experiment start time: | **12/08/2011 10:59:15** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-12005** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-12005_CS000100_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 3 of 3 11H-12005 Points 85 to 129 Quality: Good

## Sample

| | |
|---|---|
| CS000100 concentration factor | 0.564 |
| Base pKa 1 | 4.14 |
| Base pKa 2 | 10.16 |

## Sample graphs

## Other graphs

## Assay Model

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| Sample name | CS000100 | | |
| Sample by | Weight | 12/08/2011 10:00:58 | E:\T3 DATA\1108\11H-01007_CS00077_pH-metric psKa.t3r |
| Sample weight | 0.001100 g | | |
| Formula weight | 473.30 g/mol | | |
| Solubility | Unknown | 12/08/2011 10:00:58 | E:\T3 DATA\1108\11H-01007_CS00077_pH-metric psKa.t3r |
| Molecular weight | 473.30 | | |
| Individual pKa ionic environments | No | | |
| Number of pKas | 2 | | |
| Sample is a | Base | 12/08/2011 10:00:58 | E:\T3 DATA\1108\11H-01007_CS00077_pH-metric psKa.t3r |
| pKa 1 | 5.00 | | |
| pKa 2 | 9.40 | | |
| logP (XH2 2+) | -10.00 | 12/08/2011 10:00:58 | E:\T3 DATA\1108\11H-01007_CS00077_pH-metric psKa.t3r |

| | | | |
|---|---|---|---|
| Sample name: | **CS000100** | Experiment start time: | **12/08/2011 10:59:15** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-12005** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-12005_CS000100_pH-metric psKa.t3r** | | |

## Assay Model (continued)

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