# Yasuda-Shedlovsky Result

| | | | |
|---|---|---|---|
| Sample name: | **cs000093** | Experiment start time: | **24/08/2011 15:04:23** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-24009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-24009_cs000093_pH-metric psKa.t3r** | | |

## Yasuda-Shedlovsky result

| Extrapolation type | pKa 0% | SD | Intercept | Slope | $R^2$ | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|
| Yasuda-Shedlovsky | 7.67 | ±0.52 | 4.86 | 357.1041 | 0.8618 | 0.171 M | 25.0°C |

## Component assay results

| Titration | Methanol weight% | Direction | Result type | Dielectric constant | [H2O] | Ionic strength | Temperature | | psKa 1 |
|---|---|---|---|---|---|---|---|---|---|
| 11H-24009 Points 79 to 124 | 29.02 % | Up | pH-metric | 65.5 | 36.4 M | 0.177 M | 26.2°C | ☑ | 8.84 |
| 11H-24009 Points 38 to 78 | 38.42 % | Up | pH-metric | 61.6 | 30.9 M | 0.172 M | 25.2°C | ☑ | 8.99 |
| 11H-24009 Points 3 to 37 | 48.26 % | Up | pH-metric | 57.6 | 25.4 M | 0.162 M | 23.7°C | ☑ | 9.74 |

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **cs000093** | Experiment start time: | **24/08/2011 15:04:23** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-24009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-24009_cs000093_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 1 of 3 11H-24009 Points 3 to 37

## Sample

| | |
|---|---|
| cs000093 concentration factor | 0.317 |
| Base pKa 1 | 9.74 |

## Sample graphs

## Other graphs

| | | | |
|---|---|---|---|
| Sample name: | **cs000093** | Experiment start time: | **24/08/2011 15:04:23** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-24009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-24009_cs000093_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 2 of 3 11H-24009 Points 38 to 78

## Sample

| | |
|---|---|
| cs000093 concentration factor | 0.601 |
| Base pKa 1 | 8.99 |

## Sample graphs

## Other graphs

| | | | |
|---|---|---|---|
| Sample name: | **cs000093** | Experiment start time: | **24/08/2011 15:04:23** |
| Assay name: | **pH-metric psKa** | Analyst: | |
| Assay ID: | **11H-24009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-24009_cs000093_pH-metric psKa.t3r** | | |

# pH-metric psKa Titration 3 of 3 11H-24009 Points 79 to 124

## Sample

| | |
|---|---|
| cs000093 concentration factor | 0.459 |
| Base pKa 1 | 8.84 |

## Sample graphs

## Other graphs

## Assay Model

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| Sample name | cs000093 | | |
| Sample by | Weight | 24/08/2011 10:11:44 | E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r |
| Sample weight | 0.000920 g | | |
| Formula weight | 423.28 g/mol | | |
| Solubility | Unknown | 24/08/2011 10:11:44 | E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r |
| Molecular weight | 423.28 | | |
| Individual pKa ionic environments | No | | |
| Number of pKas | 1 | | |
| Sample is a | Base | | |
| pKa 1 | 9.30 | | |
| logp (XH +) | -10.00 | 24/08/2011 10:11:44 | E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r |
| logP (neutral X) | -10.00 | 24/08/2011 10:11:44 | E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r |