Yasuda-Shedlovsky Result

Sample name:	**CS000105**	Experiment start time:	**17/08/2011 12:46:10**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17008_CS000105_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	3.96	±0.07	8.15	-189.5510	0.9954	0.176 M	27.6°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-17008 Points 64 to 100	34.12 %	Up	pH-metric	62.4	33.3 M	0.186 M	28.7°C	☑	3.61
11H-17008 Points 32 to 63	47.59 %	Up	pH-metric	56.6	25.7 M	0.178 M	27.7°C	☑	3.36
11H-17008 Points 3 to 31	64.46 %	Up	pH-metric	49.1	16.8 M	0.164 M	26.4°C	☑	3.07

Graphs

Sample name:	**CS000105**	Experiment start time:	**17/08/2011 12:46:10**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17008_CS000105_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-17008 Points 3 to 31 Quality: Good

Sample

CS000105 concentration factor	1.127
Base pKa 1	3.07

Sample graphs

Other graphs

Sample name:	**CS000105**	Experiment start time:	**17/08/2011 12:46:10**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17008_CS000105_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-17008 Points 32 to 63 Quality: Good

Sample

- CS000105 concentration factor 1.019
- Base pKa 1 3.36

Sample graphs

Other graphs

Sample name:	**CS000105**	Experiment start time:	**17/08/2011 12:46:10**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17008_CS000105_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-17008 Points 64 to 100 Quality: Good

Sample

CS000105 concentration factor	0.974
Base pKa 1	3.61

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000105		
Sample by	Weight	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Sample weight	0.001120 g		
Formula weight	290.39 g/mol		
Solubility	Unknown	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Molecular weight	290.39		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	4.00	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
logp (XH +)	-10.00	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r

Sample name:	**CS000105**	Experiment start time:	**17/08/2011 12:46:10**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17008_CS000105_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logP (neutral X)	-10.00	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r