Yasuda-Shedlovsky Result

Sample name:	**CS000116**	Experiment start time:	**22/08/2011 13:43:00**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-22009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-22009_CS000116_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.78	±0.01	9.44	-305.3600	1.0000	0.177 M	26.4°C
Yasuda-Shedlovsky	9.88	±0.02	11.19	34.0750	0.9830	0.177 M	26.4°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11H-22009 Points 74 to 118	25.94 %	Up	pH-metric	66.6	38.3 M	0.186 M	27.0°C	☑	3.27	☑	).:
11H-22009 Points 37 to 73	35.68 %	Up	pH-metric	62.3	32.5 M	0.179 M	27.1°C	☑	3.03	☑	).:
11H-22009 Points 3 to 36	47.44 %	Up	pH-metric	57.5	25.8 M	0.166 M	25.2°C	☑	2.72	☑	).:

Graphs

Sample name:	**CS000116**	Experiment start time:	**22/08/2011 13:43:00**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-22009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-22009_CS000116_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-22009 Points 3 to 36 Quality: Good

Sample

CS000116 concentration factor	1.132
Base pKa 1	2.72
Base pKa 2	10.37

Sample graphs

Other graphs

Sample name:	**CS000116**	Experiment start time:	**22/08/2011 13:43:00**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-22009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-22009_CS000116_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-22009 Points 37 to 73 Quality: Good

Sample

CS000116 concentration factor	1.067
Base pKa 1	3.03
Base pKa 2	10.22

Sample graphs

Other graphs

Sample name:	**CS000116**	Experiment start time:	**22/08/2011 13:43:00**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-22009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-22009_CS000116_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-22009 Points 74 to 118 Quality: Good

Sample

CS000116 concentration factor	1.006
Base pKa 1	3.27
Base pKa 2	10.12

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000116		
Sample by	Weight	22/08/2011 13:07:31	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample weight	0.001050 g		
Formula weight	351.64 g/mol		
Solubility	Unknown	22/08/2011 13:07:31	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	351.64		
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	4.00	22/08/2011 13:07:31	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 2	9.50		

Sample name:	**CS000116**	Experiment start time:	**22/08/2011 13:43:00**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-22009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-22009_CS000116_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logP (XH2 2+)	-10.00	22/08/2011 13:07:31	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	22/08/2011 13:07:31	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00		