Yasuda-Shedlovsky Result

Sample name:	**CS000100**	Experiment start time:	**31/07/2011 12:31:58**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-31006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-31006_CS000100_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.78	±0.03	10.01	-272.5607	0.9993	0.174 M	25.7°C
Yasuda-Shedlovsky	9.97	±0.16	13.40	-131.8584	0.9011	0.174 M	25.7°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		I
11G-31006 Points 107 to 155	27.19 %	Up	pH-metric	66.4	37.6 M	0.183 M	26.1°C	☑	4.32	☑	8
11G-31006 Points 53 to 106	36.89 %	Up	pH-metric	62.0	31.8 M	0.176 M	26.0°C	☑	4.12	☑	7
11G-31006 Points 3 to 52	48.19 %	Up	pH-metric	57.2	25.4 M	0.164 M	25.0°C	☑	3.83	☑	7

Graphs

Sample name:	**CS000100**	Experiment start time:	**31/07/2011 12:31:58**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-31006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-31006_CS000100_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11G-31006 Points 3 to 52

Sample

CS000100 concentration factor	1.113
Base pKa 1	3.83
Base pKa 2	9.72

Sample graphs

Other graphs

Sample name:	**CS000100**	Experiment start time:	**31/07/2011 12:31:58**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-31006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-31006_CS000100_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11G-31006 Points 53 to 106

Sample

CS000100 concentration factor	1.073
Base pKa 1	4.12
Base pKa 2	9.71

Sample graphs

Other graphs

Sample name:	**CS000100**	Experiment start time:	**31/07/2011 12:31:58**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-31006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-31006_CS000100_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11G-31006 Points 107 to 155

Sample

CS000100 concentration factor	1.008
Base pKa 1	4.32
Base pKa 2	9.88

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000100		
Sample by	Weight	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r
Sample weight	0.001010 g		
Formula weight	473.30 g/mol		
Solubility	Unknown	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r
Molecular weight	473.30		
Individual pKa ionic environments	No		
Number of pKas	2	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r
Sample is a	Base	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r
pKa 1	4.00	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r

Sample name:	**CS000100**	Experiment start time:	**31/07/2011 12:31:58**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-31006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-31006_CS000100_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
pKa 2	8.00	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r
logP (XH2 2+)	-10.00	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r
logp (XH +)	-10.00	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r
logP (neutral X)	-10.00	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r