Yasuda-Shedlovsky Result

Sample name:	**CS000070**	Experiment start time:	**01/09/2011 14:54:39**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-01017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01017_CS000070_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	7.76	±0.12	6.43	241.3238	0.9929	0.170 M	25.0°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-01017 Points 70 to 101	40.96 %	Up	pH-metric	60.2	29.4 M	0.175 M	26.1°C	☑	8.94
11I-01017 Points 35 to 69	53.68 %	Up	pH-metric	54.6	22.4 M	0.172 M	25.1°C	☑	9.54
11I-01017 Points 3 to 34	65.56 %	Up	pH-metric	49.3	16.2 M	0.163 M	23.9°C	☑	10.10

Graphs

Sample name:	**CS000070**	Experiment start time:	**01/09/2011 14:54:39**
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Assay ID:	**11I-01017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01017_CS000070_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11I-01017 Points 3 to 34

Sample

CS000070 concentration factor	0.673
Base pKa 1	10.10

Sample graphs

Other graphs

Sample name:	**CS000070**	Experiment start time:	**01/09/2011 14:54:39**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-01017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01017_CS000070_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11I-01017 Points 35 to 69

Sample

CS000070 concentration factor	0.761
Base pKa 1	9.54

Sample graphs

Other graphs

Sample name:	**CS000070**	Experiment start time:	**01/09/2011 14:54:39**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-01017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01017_CS000070_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11I-01017 Points 70 to 101

Sample

CS000070 concentration factor	0.121
Base pKa 1	8.94

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000070		
Sample by	Weight		
Sample weight	0.000920 g		
Formula weight	384.46 g/mol		
Solubility	Unknown	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	384.46		
Individual pKa ionic environments	No		
Number of pKas	1	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r

Sample name:	**CS000070**	Experiment start time:	**01/09/2011 14:54:39**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-01017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01017_CS000070_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logP (neutral X)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r