Yasuda-Shedlovsky Result

Sample name:	**CS000165**	Experiment start time:	**09/09/2011 12:06:07**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-09006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-09006_CS000165_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	6.36		8.85	-58.2975	1.0000	0.152 M	25.6°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-09006 Points 31 to 59	62.00 %	Up	pH-metric	50.5	18.0 M	0.153 M	25.7°C	☑	6.44
11I-09006 Points 3 to 30	74.88 %	Up	pH-metric	44.3	11.6 M	0.151 M	25.5°C	☑	6.47

Graphs

Sample name:	**CS000165**	Experiment start time:	**09/09/2011 12:06:07**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-09006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-09006_CS000165_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11I-09006 Points 3 to 30 Quality: Good

Sample

CS000165 concentration factor	0.455
Base pKa 1	6.47

Sample graphs

Other graphs

Sample name:	**CS000165**	Experiment start time:	**09/09/2011 12:06:07**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-09006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-09006_CS000165_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11I-09006 Points 31 to 59 Quality: Good

Sample

CS000165 concentration factor	0.627
Base pKa 1	6.44

Sample graphs

Other graphs

Sample name:	**CS000165**	Experiment start time:	**09/09/2011 12:06:07**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-09006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-09006_CS000165_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11I-09006 Points 60 to 86 Quality: Bad

Sample

CS000165 concentration factor	0.572
Base pKa 1	8.63

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000165		
Sample by	Weight		
Sample weight	0.000680 g		
Formula weight	448.30 g/mol		
Solubility	Unknown	09/09/2011 10:01:43	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Molecular weight	448.30		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	09/09/2011 10:01:43	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
pKa 1	8.60		
logp (XH +)	-10.00	09/09/2011 10:01:43	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logP (neutral X)	-10.00	09/09/2011 10:01:43	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r