Yasuda-Shedlovsky Result

Sample name:	**CS000066**	Experiment start time:	**28/07/2011 20:51:47**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-28012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-28012_CS000066_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	2.52	±0.01	5.19	-72.2490	0.9992	0.175 M	27.4°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11G-28012 Points 67 to 104	34.96 %	Up	pH-metric	62.4	32.9 M	0.184 M	27.7°C	☑	2.52
11G-28012 Points 34 to 66	48.12 %	Up	pH-metric	56.5	25.4 M	0.177 M	27.3°C	☑	2.50
11G-28012 Points 3 to 33	64.69 %	Up	pH-metric	48.8	16.6 M	0.163 M	27.2°C	☑	2.49

Graphs

Sample name:	**CS000066**	Experiment start time:	**28/07/2011 20:51:47**
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Filename:	**E:\T3 DATA\1107\11G-28012_CS000066_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11G-28012 Points 3 to 33

Sample

CS000066 concentration factor	1.000
Base pKa 1	2.49

Sample graphs

Other graphs

Sample name:	**CS000066**	Experiment start time:	**28/07/2011 20:51:47**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-28012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-28012_CS000066_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11G-28012 Points 34 to 66

Sample

CS000066 concentration factor 1.000
Base pKa 1 2.50

Sample graphs

Other graphs

Sample name:	**CS000066**	Experiment start time:	**28/07/2011 20:51:47**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-28012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-28012_CS000066_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11G-28012 Points 67 to 104

Sample

CS000066 concentration factor	1.000
Base pKa 1	2.52

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000066		
Sample by	Weight		
Sample weight	0.000690 g		
Formula weight	381.50 g/mol		
Solubility	Unknown		
Molecular weight	381.50		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	3.00		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		