Yasuda-Shedlovsky Result

Sample name:	**CS000069**	Experiment start time:	**29/07/2011 13:26:55**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-29008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-29008_CS00069_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	6.84	±0.07	10.56	-154.1470	0.9941	0.174 M	26.6°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11G-29008 Points 85 to 126	35.58 %	Up	pH-metric	62.2	32.5 M	0.184 M	27.5°C	☑	6.59
11G-29008 Points 44 to 84	49.02 %	Up	pH-metric	56.2	24.9 M	0.176 M	26.8°C	☑	6.39
11G-29008 Points 3 to 43	65.52 %	Up	pH-metric	48.8	16.2 M	0.163 M	25.5°C	☑	6.21

Graphs

Sample name:	**CS000069**	Experiment start time:	**29/07/2011 13:26:55**
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Filename:	**E:\T3 DATA\1107\11G-29008_CS00069_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11G-29008 Points 3 to 43

Sample

CS000069 concentration factor	0.860
Base pKa 1	6.21

Sample graphs

Other graphs

Sample name:	**CS000069**	Experiment start time:	**29/07/2011 13:26:55**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-29008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-29008_CS00069_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11G-29008 Points 44 to 84

Sample

- CS000069 concentration factor 0.782
- Base pKa 1 6.39

Sample graphs

Other graphs

Sample name:	**CS000069**	Experiment start time:	**29/07/2011 13:26:55**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-29008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-29008_CS00069_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11G-29008 Points 85 to 126

Sample

CS000069 concentration factor 0.815
Base pKa 1 6.59

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000069		
Sample by	Weight		
Sample weight	0.001040 g		
Formula weight	308.34 g/mol		
Solubility	Unknown		
Molecular weight	308.34		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	4.00		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		