Yasuda-Shedlovsky Result

Sample name:	**CS000104**	Experiment start time:	**16/08/2011 13:11:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-16007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.30	±0.04	7.10	-159.7250	0.9975	0.177 M	28.0°C
Yasuda-Shedlovsky	9.68	±0.03	11.28	11.4864	0.7862	0.177 M	28.0°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11H-16007 Points 72 to 111	34.05 %	Up	pH-metric	62.4	33.4 M	0.187 M	28.8°C	☑	3.03	☑	.9
11H-16007 Points 35 to 71	47.52 %	Up	pH-metric	56.5	25.7 M	0.180 M	28.3°C	☑	2.84	☑	).(
11H-16007 Points 3 to 34	64.36 %	Up	pH-metric	48.9	16.8 M	0.166 M	27.0°C	☑	2.62	☑	).2

Graphs

Sample name:	**CS000104**	Experiment start time:	**16/08/2011 13:11:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-16007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-16007 Points 3 to 34 Quality: Good

Sample

CS000104 concentration factor	1.220
Base pKa 1	2.62
Base pKa 2	10.28

Sample graphs

Other graphs

Sample name:	**CS000104**	Experiment start time:	**16/08/2011 13:11:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-16007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-16007 Points 35 to 71 Quality: Good

Sample

CS000104 concentration factor	1.167
Base pKa 1	2.84
Base pKa 2	10.09

Sample graphs

Other graphs

Sample name:	**CS000104**	Experiment start time:	**16/08/2011 13:11:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-16007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-16007 Points 72 to 111 Quality: Good

Sample

CS000104 concentration factor	1.109
Base pKa 1	3.03
Base pKa 2	9.93

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000104		
Sample by	Weight	16/08/2011 12:08:32	E:\T3 DATA\1108\11H-03011_CS000037_pH-metric psKa.t3r
Sample weight	0.000930 g		
Formula weight	351.64 g/mol		
Solubility	Unknown	16/08/2011 12:08:32	E:\T3 DATA\1108\11H-03011_CS000037_pH-metric psKa.t3r
Molecular weight	351.64		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base	16/08/2011 12:08:32	E:\T3 DATA\1108\11H-03011_CS000037_pH-metric psKa.t3r
pKa 1	4.60		
pKa 2	9.00		
logP (XH2 2+)	-10.00	16/08/2011 12:08:32	E:\T3 DATA\1108\11H-03011_CS000037_pH-metric psKa.t3r

Sample name:	**CS000104**	Experiment start time:	**16/08/2011 13:11:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-16007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH +)	-10.00		
logP (neutral X)	-10.00		