Yasuda-Shedlovsky Result

Sample name:	**CS000096**	Experiment start time:	**20/08/2011 15:45:48**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-20013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-20013_CS000096_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.34	±0.04	17.50	-963.8761	0.9761	0.188 M	27.6°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-20013 Points 82 to 133	22.56 %	Up	pH-metric	76.3	43.7 M	0.194 M	28.2°C	☑	3.23
11H-20013 Points 39 to 81	30.48 %	Up	pH-metric	75.9	39.5 M	0.189 M	27.9°C	☑	3.20
11H-20013 Points 3 to 38	39.93 %	Up	pH-metric	75.5	34.5 M	0.179 M	26.7°C	☑	3.20

Graphs

Sample name:	**CS000096**	Experiment start time:	**20/08/2011 15:45:48**
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Filename:	**E:\T3 DATA\1108\11H-20013_CS000096_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-20013 Points 3 to 38

Sample

CS000096 concentration factor	0.484
Base pKa 1	3.20

Sample graphs

Other graphs

Sample name:	**CS000096**	Experiment start time:	**20/08/2011 15:45:48**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-20013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-20013_CS000096_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-20013 Points 39 to 81

Sample

CS000096 concentration factor	0.682
Base pKa 1	3.20

Sample graphs

Other graphs

Sample name:	**CS000096**	Experiment start time:	**20/08/2011 15:45:48**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-20013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-20013_CS000096_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-20013 Points 82 to 133

Sample

CS000096 concentration factor 0.758
Base pKa 1 3.23

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000096		
Sample by	Weight	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample weight	0.000500 g		
Formula weight	419.89 g/mol		
Solubility	Unknown	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	419.89		
Individual pKa ionic environments	No		
Number of pKas	1	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r

Sample name:	**CS000096**	Experiment start time:	**20/08/2011 15:45:48**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-20013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-20013_CS000096_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH +)	-10.00	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r