Yasuda-Shedlovsky Result

Sample name:	**CS000100**	Experiment start time:	**04/08/2011 17:25:38**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-04012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-04012_CS000100_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	4.94	±0.23	41.11	-2686.6770	0.9320	0.186 M	26.5°C
Yasuda-Shedlovsky	9.63	±0.07	68.31	-4443.0385	0.9973	0.186 M	26.5°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11H-04012 Points 86 to 129	24.03 %	Up	pH-metric	76.4	42.9 M	0.195 M	27.5°C	✓	4.37	✓	8.54
11H-04012 Points 41 to 85	31.70 %	Up	pH-metric	76.3	38.9 M	0.189 M	26.6°C	✓	4.25	✓	8.50
11H-04012 Points 3 to 40	42.37 %	Up	pH-metric	75.7	33.2 M	0.174 M	25.3°C	✓	4.11	✓	8.09

Graphs

Sample name:	**CS000100**	Experiment start time:	**04/08/2011 17:25:38**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-04012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-04012_CS000100_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-04012 Points 3 to 40

Sample

CS000100 concentration factor	0.286
Base pKa 1	4.11
Base pKa 2	8.09

Sample graphs

Other graphs

Sample name:	**CS000100**	Experiment start time:	**04/08/2011 17:25:38**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-04012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-04012_CS000100_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-04012 Points 41 to 85

Sample

CS000100 concentration factor	0.390
Base pKa 1	4.25
Base pKa 2	8.50

Sample graphs

Other graphs

Sample name:	**CS000100**	Experiment start time:	**04/08/2011 17:25:38**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-04012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-04012_CS000100_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-04012 Points 86 to 129

Sample

CS000100 concentration factor	0.462
Base pKa 1	4.37
Base pKa 2	8.54

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000100		
Sample by	Weight		
Sample weight	0.000930 g		
Formula weight	473.30 g/mol		
Solubility	Unknown		
Molecular weight	473.30		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base		
pKa 1	4.00		
pKa 2	8.00		
logP (XH2 2+)	-10.00		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		