Yasuda-Shedlovsky Result

Sample name:	**CS000104**	Experiment start time:	**17/08/2011 18:30:16**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17013_CS000104_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.56	±0.10	28.90	-1840.6730	0.9782	0.193 M	26.5°C
Yasuda-Shedlovsky	9.46	±0.00	3.51	599.8500	0.9999	0.193 M	26.5°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11H-17013 Points 83 to 128	24.93 %	Up	pH-metric	76.6	42.5 M	0.201 M	26.9°C	✓	3.27	✓	.7
11H-17013 Points 40 to 82	33.07 %	Up	pH-metric	76.1	38.2 M	0.196 M	26.8°C	✓	3.10	✓	.8
11H-17013 Points 3 to 39	45.09 %	Up	pH-metric	75.1	31.7 M	0.181 M	25.9°C	✓	2.91	✓	0.0

Graphs

Sample name:	**CS000104**	Experiment start time:	**17/08/2011 18:30:16**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17013_CS000104_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-17013 Points 3 to 39 Quality: Good

Sample

CS000104 concentration factor	0.916
Base pKa 1	2.91
Base pKa 2	10.00

Sample graphs

Other graphs

Sample name:	**CS000104**	Experiment start time:	**17/08/2011 18:30:16**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17013_CS000104_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-17013 Points 40 to 82 Quality: Good

Sample

CS000104 concentration factor	0.902
Base pKa 1	3.10
Base pKa 2	9.81

Sample graphs

Other graphs

Sample name:	**CS000104**	Experiment start time:	**17/08/2011 18:30:16**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17013_CS000104_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-17013 Points 83 to 128 Quality: Good

Sample

CS000104 concentration factor	0.911
Base pKa 1	3.27
Base pKa 2	9.72

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000104	17/08/2011 18:30:04	E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r
Sample by	Weight	17/08/2011 18:30:04	E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r
Sample weight	0.001020 g		
Formula weight	351.64 g/mol	17/08/2011 18:30:04	E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r
Solubility	Unknown	17/08/2011 18:30:04	E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r
Molecular weight	351.64		
Individual pKa ionic environments	No		
Number of pKas	2	17/08/2011 18:30:04	E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r

Sample name:	**CS000104**	Experiment start time:	**17/08/2011 18:30:16**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17013_CS000104_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
Sample is a	Base	17/08/2011 18:30:04	E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r
pKa 1	4.60	17/08/2011 18:30:04	E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r
pKa 2	9.00	17/08/2011 18:30:04	E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r
logP (XH2 2+)	-10.00	17/08/2011 18:30:04	E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r
logp (XH +)	-10.00	17/08/2011 18:30:04	E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r
logP (neutral X)	-10.00	17/08/2011 18:30:04	E:\T3 DATA\1108\11H-16007_CS000104_pH-metric psKa.t3r