Yasuda-Shedlovsky Result

Sample name:	**CS000032**	Experiment start time:	**03/08/2011 17:08:01**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-03009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-03009_CS000032_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.93	±0.20	43.40	-2938.1100	0.9557	0.188 M	26.9°C
Yasuda-Shedlovsky	9.28	±0.06	-7.55	1446.3300	0.9856	0.188 M	26.9°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11H-03009 Points 87 to 138	23.92 %	Up	pH-metric	76.7	43.0 M	0.195 M	26.9°C	✓	3.49	✓	.6
11H-03009 Points 43 to 86	31.10 %	Up	pH-metric	76.2	39.2 M	0.190 M	27.0°C	✓	3.15	✓	.8
11H-03009 Points 3 to 42	40.51 %	Up	pH-metric	75.4	34.1 M	0.178 M	26.8°C	✓	2.93	✓	0.0

Graphs

Sample name:	**CS000032**	Experiment start time:	**03/08/2011 17:08:01**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-03009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-03009_CS000032_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-03009 Points 3 to 42 Quality: Good

Sample

CS000032 concentration factor	0.784
Base pKa 1	2.93
Base pKa 2	10.09

Sample graphs

Other graphs

Sample name:	**CS000032**	Experiment start time:	**03/08/2011 17:08:01**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-03009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-03009_CS000032_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-03009 Points 43 to 86 Quality: Good

Sample

CS000032 concentration factor	0.853
Base pKa 1	3.15
Base pKa 2	9.87

Sample graphs

Other graphs

Sample name:	**CS000032**	Experiment start time:	**03/08/2011 17:08:01**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-03009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-03009_CS000032_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-03009 Points 87 to 138 Quality: Good

Sample

CS000032 concentration factor	0.832
Base pKa 1	3.49
Base pKa 2	9.67

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000032		
Sample by	Weight		
Sample weight	0.000900 g		
Formula weight	352.39 g/mol		
Solubility	Unknown	03/08/2011 12:08:07	E:\T3 DATA\1107\11G-26012_CS000053_Fast UV psKa.t3r
Molecular weight	352.39		
Individual pKa ionic environments	No		
Number of pKas	2	03/08/2011 12:08:07	E:\T3 DATA\1107\11G-26012_CS000053_Fast UV psKa.t3r
Sample is a	Base	03/08/2011 12:08:07	E:\T3 DATA\1107\11G-26012_CS000053_Fast UV psKa.t3r
pKa 1	4.00	03/08/2011 12:08:07	E:\T3 DATA\1107\11G-26012_CS000053_Fast UV psKa.t3r
pKa 2	10.00	03/08/2011 12:08:07	E:\T3 DATA\1107\11G-26012_CS000053_Fast UV psKa.t3r
logP (XH2 2+)	-10.00	03/08/2011 12:08:07	E:\T3 DATA\1107\11G-26012_CS000053_Fast UV psKa.t3r
logp (XH +)	-10.00	03/08/2011 12:08:07	E:\T3 DATA\1107\11G-26012_CS000053_Fast UV psKa.t3r

Sample name:	**CS000032**	Experiment start time:	**03/08/2011 17:08:01**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-03009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-03009_CS000032_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logP (neutral X)	-10.00	03/08/2011 12:08:07	E:\T3 DATA\1107\11G-26012_CS000053_Fast UV psKa.t3r