Yasuda-Shedlovsky Result

Sample name:	**cs000085**	Experiment start time:	**17/08/2011 19:40:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17014_cs000085_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	2.52	±0.02	25.40	-1650.0433	0.9984	0.194 M	26.3°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-17014 Points 85 to 137	24.61 %	Up	pH-metric	77.1	42.7 M	0.201 M	25.4°C	☑	2.37
11H-17014 Points 40 to 84	32.21 %	Up	pH-metric	76.1	38.6 M	0.197 M	26.9°C	☑	2.14
11H-17014 Points 3 to 39	42.44 %	Up	pH-metric	75.3	33.1 M	0.185 M	26.4°C	☑	1.96

Graphs

Sample name:	**cs000085**	Experiment start time:	**17/08/2011 19:40:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17014_cs000085_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-17014 Points 3 to 39 Quality: Good

Sample

cs000085 concentration factor	1.000
Base pKa 1	1.96

Sample graphs

Other graphs

Sample name:	**cs000085**	Experiment start time:	**17/08/2011 19:40:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17014_cs000085_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-17014 Points 40 to 84 Quality: Good

Sample

cs000085 concentration factor 1.000
Base pKa 1 2.14

Sample graphs

Other graphs

Sample name:	**cs000085**	Experiment start time:	**17/08/2011 19:40:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17014_cs000085_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-17014 Points 85 to 137 Quality: Good

Sample

cs000085 concentration factor	1.000
Base pKa 1	2.37

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000085	17/08/2011 19:40:34	E:\T3 DATA\1108\11H-16015_cs000085_pH-metric psKa.t3r
Sample by	Weight	17/08/2011 19:40:34	E:\T3 DATA\1108\11H-16015_cs000085_pH-metric psKa.t3r
Sample weight	0.000970 g		
Formula weight	337.34 g/mol	17/08/2011 19:40:34	E:\T3 DATA\1108\11H-16015_cs000085_pH-metric psKa.t3r
Solubility	Unknown	17/08/2011 19:40:34	E:\T3 DATA\1108\11H-16015_cs000085_pH-metric psKa.t3r
Molecular weight	337.34		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	17/08/2011 19:40:34	E:\T3 DATA\1108\11H-16015_cs000085_pH-metric psKa.t3r
pKa 1	3.00		

Sample name:	**cs000085**	Experiment start time:	**17/08/2011 19:40:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17014_cs000085_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH +)	-10.00	17/08/2011 19:40:34	E:\T3 DATA\1108\11H-16015_cs000085_pH-metric psKa.t3r
logP (neutral X)	-10.00		