Yasuda-Shedlovsky Result

Sample name:	**CS000080**	Experiment start time:	**01/08/2011 12:15:01**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-01005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	6.45	±0.00	32.58	-1940.8260	1.0000	0.184 M	22.1°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-01005 Points 78 to 119	25.09 %	Up	pH-metric	77.8	42.4 M	0.193 M	23.6°C	☑	6.00
11H-01005 Points 38 to 77	33.06 %	Up	pH-metric	77.5	38.2 M	0.187 M	22.6°C	☑	5.97
11H-01005 Points 3 to 37	43.55 %	Up	pH-metric	77.3	32.6 M	0.173 M	20.2°C	☑	5.96

Graphs

Sample name:	**CS000080**	Experiment start time:	**01/08/2011 12:15:01**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-01005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-01005 Points 3 to 37 Quality: Good

Sample

CS000080 concentration factor	0.898
Base pKa 1	5.96

Sample graphs

Other graphs

Sample name:	**CS000080**	Experiment start time:	**01/08/2011 12:15:01**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-01005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-01005 Points 38 to 77 Quality: Good

Sample

CS000080 concentration factor	0.803
Base pKa 1	5.97

Sample graphs

Other graphs

Sample name:	**CS000080**	Experiment start time:	**01/08/2011 12:15:01**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-01005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-01005 Points 78 to 119 Quality: Good

Sample

CS000080 concentration factor	0.638
Base pKa 1	6.00

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000080		
Sample by	Weight		
Sample weight	0.001010 g		
Formula weight	340.34 g/mol		
Solubility	Unknown		
Molecular weight	340.34		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	4.00		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		