Yasuda-Shedlovsky Result

Sample name:	**CS000080**	Experiment start time:	**09/08/2011 11:09:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-09005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09005_CS000080_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	6.54	±0.13	10.03	-135.8228	0.9713	0.174 M	27.0°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-09005 Points 84 to 121	34.79 %	Up	pH-metric	62.4	33.0 M	0.183 M	28.0°C	☑	6.37
11H-09005 Points 43 to 83	47.64 %	Up	pH-metric	56.8	25.7 M	0.176 M	26.9°C	☑	6.17
11H-09005 Points 3 to 42	64.69 %	Up	pH-metric	49.0	16.6 M	0.163 M	26.2°C	☑	6.06

Graphs

Sample name:	**CS000080**	Experiment start time:	**09/08/2011 11:09:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-09005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09005_CS000080_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-09005 Points 3 to 42

Sample

CS000080 concentration factor	0.826
Base pKa 1	6.06

Sample graphs

Other graphs

Sample name:	**CS000080**	Experiment start time:	**09/08/2011 11:09:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-09005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09005_CS000080_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-09005 Points 43 to 83

Sample

CS000080 concentration factor	0.814
Base pKa 1	6.17

Sample graphs

Other graphs

Sample name:	**CS000080**	Experiment start time:	**09/08/2011 11:09:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-09005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09005_CS000080_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-09005 Points 84 to 121

Sample

CS000080 concentration factor	0.702
Base pKa 1	6.37

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000080		
Sample by	Weight	09/08/2011 10:19:25	E:\T3 DATA\1108\11H-08011_CS000074_pH-metric psKa.t3r
Sample weight	0.001010 g		
Formula weight	340.30 g/mol		
Solubility	Unknown	09/08/2011 10:19:25	E:\T3 DATA\1108\11H-08011_CS000074_pH-metric psKa.t3r
Molecular weight	340.30		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	09/08/2011 10:19:25	E:\T3 DATA\1108\11H-08011_CS000074_pH-metric psKa.t3r
pKa 1	4.24	09/08/2011 10:19:25	E:\T3 DATA\1108\11H-08011_CS000074_pH-metric psKa.t3r
logp (XH +)	-10.00	09/08/2011 10:19:25	E:\T3 DATA\1108\11H-08011_CS000074_pH-metric psKa.t3r

Sample name:	**CS000080**	Experiment start time:	**09/08/2011 11:09:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-09005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09005_CS000080_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logP (neutral X)	-10.00	09/08/2011 10:19:25	E:\T3 DATA\1108\11H-08011_CS000074_pH-metric psKa.t3r