Yasuda-Shedlovsky Result

Sample name:	**CS00064**	Experiment start time:	**05/08/2011 22:11:50**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-05025**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-05025_CS00064_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.04	±0.04	8.58	-217.7642	0.9989	0.174 M	26.7°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-05025 Points 74 to 116	33.05 %	Up	pH-metric	63.4	34.0 M	0.183 M	27.2°C	☑	3.62
11H-05025 Points 37 to 73	46.98 %	Up	pH-metric	57.2	26.0 M	0.176 M	26.7°C	☑	3.34
11H-05025 Points 3 to 36	64.77 %	Up	pH-metric	49.0	16.6 M	0.163 M	26.0°C	☑	2.93

Graphs

Sample name:	**CS00064**	Experiment start time:	**05/08/2011 22:11:50**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-05025**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-05025_CS00064_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-05025 Points 3 to 36

Sample

CS00064 concentration factor	1.000
Base pKa 1	2.93

Sample graphs

Other graphs

Sample name:	**CS00064**	Experiment start time:	**05/08/2011 22:11:50**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-05025**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-05025_CS00064_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-05025 Points 37 to 73

Sample

CS00064 concentration factor	1.000
Base pKa 1	3.34

Sample graphs

Other graphs

Sample name:	**CS00064**	Experiment start time:	**05/08/2011 22:11:50**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-05025**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-05025_CS00064_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-05025 Points 74 to 116

Sample

CS00064 concentration factor	1.000
Base pKa 1	3.62

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS00064	05/08/2011 22:09:15	E:\T3 DATA\1107\11H-02009_CS00064_pH-metric psKa.t3r
Sample by	Weight	05/08/2011 22:09:15	E:\T3 DATA\1107\11H-02009_CS00064_pH-metric psKa.t3r
Sample weight	0.001470 g		
Formula weight	329.38 g/mol	05/08/2011 22:09:15	E:\T3 DATA\1107\11H-02009_CS00064_pH-metric psKa.t3r
Solubility	Unknown	05/08/2011 22:09:15	E:\T3 DATA\1107\11H-02009_CS00064_pH-metric psKa.t3r
Molecular weight	329.38		
Individual pKa ionic environments	No		
Number of pKas	1	05/08/2011 22:09:15	E:\T3 DATA\1107\11H-02009_CS00064_pH-metric psKa.t3r
Sample is a	Base	05/08/2011 22:09:15	E:\T3 DATA\1107\11H-02009_CS00064_pH-metric psKa.t3r

Sample name:	**CS00064**	Experiment start time:	**05/08/2011 22:11:50**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-05025**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-05025_CS00064_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
pKa 1	4.00	05/08/2011 22:09:15	E:\T3 DATA\1107\11H-02009_CS00064_pH-metric psKa.t3r
logp (XH +)	-10.00	05/08/2011 22:09:15	E:\T3 DATA\1107\11H-02009_CS00064_pH-metric psKa.t3r
logP (neutral X)	-10.00	05/08/2011 22:09:15	E:\T3 DATA\1107\11H-02009_CS00064_pH-metric psKa.t3r