Yasuda-Shedlovsky Result

Sample name:	**CS000092**	Experiment start time:	**17/08/2011 10:55:03**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17006_CS000092_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.16	±0.04	6.64	-134.6340	0.9977	0.176 M	27.2°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-17006 Points 63 to 97	34.74 %	Up	pH-metric	62.2	33.0 M	0.185 M	28.6°C	☑	2.97
11H-17006 Points 32 to 62	48.23 %	Up	pH-metric	56.4	25.3 M	0.178 M	27.5°C	☑	2.83
11H-17006 Points 3 to 31	65.04 %	Up	pH-metric	49.0	16.5 M	0.164 M	25.6°C	☑	2.68

Graphs

Sample name:	**CS000092**	Experiment start time:	**17/08/2011 10:55:03**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17006_CS000092_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-17006 Points 3 to 31 Quality: Good

Sample

- CS000092 concentration factor 1.268
- Base pKa 1 2.68

Sample graphs

Other graphs

Sample name:	**CS000092**	Experiment start time:	**17/08/2011 10:55:03**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17006_CS000092_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-17006 Points 32 to 62 Quality: Good

Sample

- CS000092 concentration factor 1.126
- Base pKa 1 2.83

Sample graphs

Other graphs

Sample name:	**CS000092**	Experiment start time:	**17/08/2011 10:55:03**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17006_CS000092_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-17006 Points 63 to 97 Quality: Good

Sample

CS000092 concentration factor 0.911
Base pKa 1 2.97

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000092		
Sample by	Weight	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Sample weight	0.001050 g		
Formula weight	345.40 g/mol		
Solubility	Unknown	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Molecular weight	345.40		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	4.00	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
logp (XH +)	-10.00	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r

Sample name:	**CS000092**	Experiment start time:	**17/08/2011 10:55:03**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17006_CS000092_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logP (neutral X)	-10.00	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r