Yasuda-Shedlovsky Result

Sample name:	**CS000096**	Experiment start time:	**17/08/2011 11:46:41**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17007_CS000096_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.23	±0.06	7.94	-229.6355	0.9979	0.176 M	27.8°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-17007 Points 64 to 98	34.38 %	Up	pH-metric	62.3	33.2 M	0.185 M	28.8°C	☑	2.75
11H-17007 Points 32 to 63	47.95 %	Up	pH-metric	56.3	25.5 M	0.178 M	28.1°C	☑	2.43
11H-17007 Points 3 to 31	64.83 %	Up	pH-metric	48.8	16.6 M	0.164 M	26.6°C	☑	2.03

Graphs

Sample name:	**CS000096**	Experiment start time:	**17/08/2011 11:46:41**
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Assay ID:	**11H-17007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17007_CS000096_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-17007 Points 3 to 31

Sample

CS000096 concentration factor	2.347
Base pKa 1	2.03

Sample graphs

Other graphs

Sample name:	**CS000096**	Experiment start time:	**17/08/2011 11:46:41**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17007_CS000096_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-17007 Points 32 to 63

Sample

- CS000096 concentration factor 1.648
- Base pKa 1 2.43

Sample graphs

Other graphs

Sample name:	**CS000096**	Experiment start time:	**17/08/2011 11:46:41**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-17007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-17007_CS000096_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-17007 Points 64 to 98

Sample

CS000096 concentration factor 1.249
Base pKa 1 2.75

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000096		
Sample by	Weight	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Sample weight	0.000990 g		
Formula weight	419.89 g/mol		
Solubility	Unknown	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Molecular weight	419.89		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	3.30		
logp (XH +)	-10.00	17/08/2011 10:14:43	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
logP (neutral X)	-10.00		