Yasuda-Shedlovsky Result

Sample name:	**CS000065**	Experiment start time:	**28/08/2011 13:21:26**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28006_CS000065_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	6.65	±0.01	19.56	-868.7570	0.9995	0.190 M	27.0°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-28006 Points 90 to 137	26.18 %	Up	pH-metric	76.3	41.8 M	0.197 M	27.5°C	☑	6.56
11H-28006 Points 45 to 89	34.35 %	Up	pH-metric	75.9	37.5 M	0.192 M	27.1°C	☑	6.53
11H-28006 Points 3 to 44	44.74 %	Up	pH-metric	75.0	31.8 M	0.180 M	26.4°C	☑	6.47

Graphs

Sample name:	**CS000065**	Experiment start time:	**28/08/2011 13:21:26**
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Filename:	**E:\T3 DATA\1108\11H-28006_CS000065_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-28006 Points 3 to 44

Sample

CS000065 concentration factor	0.955
Base pKa 1	6.47

Sample graphs

Other graphs

Sample name:	**CS000065**	Experiment start time:	**28/08/2011 13:21:26**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28006_CS000065_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-28006 Points 45 to 89

Sample

CS000065 concentration factor	0.979
Base pKa 1	6.53

Sample graphs

Other graphs

Sample name:	**CS000065**	Experiment start time:	**28/08/2011 13:21:26**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28006_CS000065_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-28006 Points 90 to 137

Sample

- CS000065 concentration factor 1.074
- Base pKa 1 6.56

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000065		
Sample by	Weight		
Sample weight	0.000960 g		
Formula weight	475.92 g/mol		
Solubility	Unknown		
Molecular weight	475.92		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	6.00		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		