Yasuda-Shedlovsky Result

Sample name:	**CS000142**	Experiment start time:	**28/08/2011 19:12:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28011_CS000142_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	4.99	±0.00	22.98	-1254.9693	0.9999	0.190 M	28.7°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-28011 Points 80 to 123	26.19 %	Up	pH-metric	75.8	41.8 M	0.197 M	29.1°C	☑	4.79
11H-28011 Points 40 to 79	34.43 %	Up	pH-metric	75.3	37.4 M	0.192 M	28.8°C	☑	4.74
11H-28011 Points 3 to 39	44.90 %	Up	pH-metric	74.4	31.7 M	0.180 M	28.1°C	☑	4.61

Graphs

Sample name:	**CS000142**	Experiment start time:	**28/08/2011 19:12:59**
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Filename:	**E:\T3 DATA\1108\11H-28011_CS000142_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-28011 Points 3 to 39

Sample

- CS000142 concentration factor 0.960
- Base pKa 1 4.61

Sample graphs

Other graphs

Sample name:	**CS000142**	Experiment start time:	**28/08/2011 19:12:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28011_CS000142_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-28011 Points 40 to 79

Sample

CS000142 concentration factor	1.001
Base pKa 1	4.74

Sample graphs

Other graphs

Sample name:	**CS000142**	Experiment start time:	**28/08/2011 19:12:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28011_CS000142_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-28011 Points 80 to 123

Sample

- CS000142 concentration factor 0.983
- Base pKa 1 4.79

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000142		
Sample by	Weight		
Sample weight	0.000960 g		
Formula weight	295.30 g/mol		
Solubility	Unknown		
Molecular weight	295.30		
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		