Yasuda-Shedlovsky Result

Sample name:	**CS000070**	Experiment start time:	**28/08/2011 14:35:16**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28007_CS000070_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	8.49	±0.02	-11.50	1690.4541	0.9993	0.190 M	27.1°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-28007 Points 83 to 129	26.25 %	Up	pH-metric	76.2	41.8 M	0.197 M	27.7°C	☑	9.06
11H-28007 Points 41 to 82	34.49 %	Up	pH-metric	75.9	37.4 M	0.192 M	27.1°C	☑	9.21
11H-28007 Points 3 to 40	44.78 %	Up	pH-metric	75.0	31.8 M	0.181 M	26.4°C	☑	9.54

Graphs

Sample name:	**CS000070**	Experiment start time:	**28/08/2011 14:35:16**
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Filename:	**E:\T3 DATA\1108\11H-28007_CS000070_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-28007 Points 3 to 40

Sample

- CS000070 concentration factor 0.413
- Base pKa 1 9.54

Sample graphs

Other graphs

Sample name:	**CS000070**	Experiment start time:	**28/08/2011 14:35:16**
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Assay ID:	**11H-28007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28007_CS000070_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-28007 Points 41 to 82

Sample

CS000070 concentration factor	0.434
Base pKa 1	9.21

Sample graphs

Other graphs

Sample name:	**CS000070**	Experiment start time:	**28/08/2011 14:35:16**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28007_CS000070_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-28007 Points 83 to 129

Sample

CS000070 concentration factor	0.500
Base pKa 1	9.06

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000070		
Sample by	Weight		
Sample weight	0.000990 g		
Formula weight	384.46 g/mol		
Solubility	Unknown		
Molecular weight	384.46		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	4.00		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		