Yasuda-Shedlovsky Result

Sample name:	**CS000095**	Experiment start time:	**04/08/2011 16:16:44**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-04011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-04011_CS000095_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	2.92	±0.00	7.61	-229.7430	0.9977	0.188 M	26.1°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-04011 Points 73 to 112	23.66 %	Up	pH-metric	76.7	43.1 M	0.195 M	26.7°C	☑	2.98
11H-04011 Points 36 to 72	30.75 %	Up	pH-metric	76.2	39.4 M	0.190 M	27.0°C	☑	2.99
11H-04011 Points 3 to 35	40.26 %	Up	pH-metric	76.1	34.3 M	0.178 M	24.8°C	☑	3.05

Graphs

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Assay ID:	**11H-04011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-04011_CS000095_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-04011 Points 3 to 35

Sample

CS000095 concentration factor	0.547
Base pKa 1	3.05

Sample graphs

Other graphs

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Sample name:	**CS000095**	Experiment start time:	**04/08/2011 16:16:44**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-04011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-04011_CS000095_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-04011 Points 36 to 72

Sample

CS000095 concentration factor	0.771
Base pKa 1	2.99

Sample graphs

Other graphs

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Sample name:	**CS000095**	Experiment start time:	**04/08/2011 16:16:44**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-04011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-04011_CS000095_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-04011 Points 73 to 112

Sample

CS000095 concentration factor	1.000
Base pKa 1	2.98

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000095		
Sample by	Weight		
Sample weight	0.000950 g		
Formula weight	369.40 g/mol		
Solubility	Unknown		
Molecular weight	369.40		
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		

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