Yasuda-Shedlovsky Result

Sample name:	**CS000032**	Experiment start time:	**10/08/2011 19:36:40**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-10015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-10015_CS000032_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.86	±0.15	7.92	-180.5110	0.9860	0.171 M	26.7°C
Yasuda-Shedlovsky	9.50	±0.00	10.04	93.5059	1.0000	0.171 M	26.7°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11H-10015 Points 80 to 126	39.85 %	Down	pH-metric	60.7	30.1 M	0.182 M	26.2°C	☑	3.50	☑	).:
11H-10015 Points 40 to 79	58.04 %	Down	pH-metric	51.7	20.1 M	0.173 M	27.8°C	☑	3.06	☑	).5
11H-10015 Points 3 to 39	71.83 %	Down	pH-metric	45.6	13.1 M	0.157 M	26.1°C	☑	2.88	☑	).9

Graphs

Sample name:	**CS000032**	Experiment start time:	**10/08/2011 19:36:40**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-10015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-10015_CS000032_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-10015 Points 3 to 39 Quality: Good

Sample

CS000032 concentration factor	1.466
Base pKa 1	2.88
Base pKa 2	10.97

Sample graphs

Other graphs

Sample name:	**CS000032**	Experiment start time:	**10/08/2011 19:36:40**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-10015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-10015_CS000032_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-10015 Points 40 to 79 Quality: Good

Sample

CS000032 concentration factor	1.327
Base pKa 1	3.06
Base pKa 2	10.55

Sample graphs

Other graphs

Sample name:	**CS000032**	Experiment start time:	**10/08/2011 19:36:40**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-10015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-10015_CS000032_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-10015 Points 80 to 126 Quality: Good

Sample

CS000032 concentration factor	1.211
Base pKa 1	3.50
Base pKa 2	10.10

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000032	10/08/2011 19:36:24	E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r
Sample by	Weight		
Sample weight	0.000900 g		
Formula weight	473.30 g/mol	10/08/2011 19:36:24	E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r
Solubility	Unknown	10/08/2011 19:36:24	E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r
Molecular weight	352.40		
Individual pKa ionic environments	No		
Number of pKas	2	10/08/2011 19:36:24	E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r
Sample is a	Base	10/08/2011 19:36:24	E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r
pKa 1	4.00	10/08/2011 19:36:24	E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r
pKa 2	8.00	10/08/2011 19:36:24	E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r
logP (XH2 2+)	-10.00	10/08/2011 19:36:24	E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r

Sample name:	**CS000032**	Experiment start time:	**10/08/2011 19:36:40**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-10015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-10015_CS000032_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH +)	-10.00	10/08/2011 19:36:24	E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r
logP (neutral X)	-10.00	10/08/2011 19:36:24	E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r