Yasuda-Shedlovsky Result

Sample name:	**CS000041**	Experiment start time:	**23/07/2011 11:50:15**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-23005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-23005_CS000041_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.04	±0.07	7.49	-133.0690	0.9936	0.156 M	25.7°C
Yasuda-Shedlovsky	7.13	±0.05	9.00	-10.0921	0.6636	0.156 M	25.7°C

Component assay results

Titration	MDM-mix weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11G-23005 Points 66 to 101	42.14 %	Up	pH-metric	55.8	30.2 M	0.159 M	27.0°C	☑	3.63	☑	.3
11G-23005 Points 34 to 65	52.95 %	Up	pH-metric	50.0	24.2 M	0.157 M	26.0°C	☑	3.46	☑	.4
11G-23005 Points 3 to 33	55.06 %	Up	pH-metric	48.9	23.0 M	0.153 M	24.1°C	☑	3.39	☑	.4

Graphs

Sample name:	**CS000041**	Experiment start time:	**23/07/2011 11:50:15**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-23005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-23005_CS000041_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11G-23005 Points 3 to 33

Sample

CS000041 concentration factor	0.729
Base pKa 1	3.39
Base pKa 2	7.44

Sample graphs

Other graphs

Sample name:	**CS000041**	Experiment start time:	**23/07/2011 11:50:15**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-23005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-23005_CS000041_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11G-23005 Points 34 to 65

Sample

CS000041 concentration factor	0.633
Base pKa 1	3.46
Base pKa 2	7.40

Sample graphs

Other graphs

Sample name:	**CS000041**	Experiment start time:	**23/07/2011 11:50:15**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-23005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-23005_CS000041_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11G-23005 Points 66 to 101

Sample

CS000041 concentration factor	0.636
Base pKa 1	3.63
Base pKa 2	7.34

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000041	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
Sample by	Weight	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
Sample weight	0.000280 g		
Formula weight	341.39 g/mol	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
Solubility	Unknown	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
Molecular weight	341.39		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base		
pKa 1	4.00		
pKa 2	8.00		

Sample name:	**CS000041**	Experiment start time:	**23/07/2011 11:50:15**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-23005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-23005_CS000041_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logP (XH2 2+)	-10.00	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
logp (XH +)	-10.00	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
logP (neutral X)	-10.00		