Yasuda-Shedlovsky Result

Sample name:	**CS000081**	Experiment start time:	**10/08/2011 20:50:28**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-10016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-10016_CS000081_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature
11H-10016 Points 80 to 122	40.84 %	Down	pH-metric	60.4	29.5 M	0.179 M	25.6°C
11H-10016 Points 40 to 79	58.71 %	Down	pH-metric	52.2	19.8 M	0.170 M	25.3°C
11H-10016 Points 3 to 39	72.28 %	Down	pH-metric	45.8	12.9 M	0.154 M	24.7°C

Graphs

Sample name:	**CS000081**	Experiment start time:	**10/08/2011 20:50:28**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-10016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-10016_CS000081_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-10016 Points 3 to 39

Sample

CS000081 concentration factor 1.000

Sample graphs

Other graphs

Sample name:	**CS000081**	Experiment start time:	**10/08/2011 20:50:28**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-10016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-10016_CS000081_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-10016 Points 40 to 79

Sample

CS000081 concentration factor 1.000

Sample graphs

Other graphs

Sample name:	**CS000081**	Experiment start time:	**10/08/2011 20:50:28**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-10016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-10016_CS000081_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-10016 Points 80 to 122

Sample

CS000081 concentration factor 1.000

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000081	10/08/2011 20:50:13	E:\T3 DATA\1108\11H-09017_CS000081_Fast UV psKa.t3r
Sample by	Weight		
Sample weight	0.000840 g		
Formula weight	473.30 g/mol	10/08/2011 20:50:13	E:\T3 DATA\1108\11H-09017_CS000081_Fast UV psKa.t3r
Solubility	Unknown	10/08/2011 20:50:13	E:\T3 DATA\1108\11H-09017_CS000081_Fast UV psKa.t3r
Molecular weight	383.50		
Individual pKa ionic environments	No		
Number of pKas	0	10/08/2011 20:50:13	E:\T3 DATA\1108\11H-09017_CS000081_Fast UV psKa.t3r
logP (neutral X)	-10.00	10/08/2011 20:50:13	E:\T3 DATA\1108\11H-09017_CS000081_Fast UV psKa.t3r