Yasuda-Shedlovsky Result

Sample name:	**CS000160**	Experiment start time:	**07/09/2011 16:30:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07018**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07018_CS000160_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

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

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature
11I-07018 Points 105 to 156	19.90 %	Up	UV-metric pKa	77.5	45.1 M	0.207 M	25.0°C
11I-07018 Points 53 to 104	26.82 %	Up	UV-metric pKa	77.3	41.5 M	0.204 M	24.6°C
11I-07018 Points 3 to 52	35.99 %	Up	UV-metric pKa	76.2	36.6 M	0.194 M	25.6°C

Graphs

Sample name:	**CS000160**	Experiment start time:	**07/09/2011 16:30:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07018**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07018_CS000160_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-07018 Points 3 to 52

Graphs

Sample name:	**CS000160**	Experiment start time:	**07/09/2011 16:30:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07018**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07018_CS000160_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-07018 Points 53 to 104

Graphs

Sample name:	**CS000160**	Experiment start time:	**07/09/2011 16:30:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07018**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07018_CS000160_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-07018 Points 105 to 156

Graphs

Sample name:	**CS000160**	Experiment start time:	**07/09/2011 16:30:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07018**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07018_CS000160_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000160		
Sample by	Volume	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Molecular weight	451.93		
Individual pKa ionic environments	No		
Number of pKas	0		
logP (neutral X)	-10.00	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r