Table 2. Training set, experiments 1-3.

Polymer Molar Tg Exp. 1 Exp. 2 Exp. 3

fraction (K) Out  Out  Out 

of *r* dyads (K) (K) (K) (K) (K) (K)

Poly(methyl acrylate) 0.6 281 311 32 281 27 306 26

0 283 278 12 283 16 279 9

Poly(propyl acrylate) 0.6 236 237 11 236 19 238 19

Poly(*iso*propyl acrylate) 1 271 287 20 271 26 291 24

0.6 267 265 10 267 10 267 11

0 262 248 17 262 17 250 16

Poly(butyl acrylate) 0.6 219 219 9 219 13 221 9

Poly(*iso*butyl acrylate) 0.6 249 252 17 249 15 257 14

Poly(*sec*butyl acrylate) 1 253 273 21 253 27 273 21

0.6 251 252 7 251 10 250 8

0 250 235 18 250 17 233 19

Poly(*n*-penthyl acrylate) 0.6 216 215 8 216 9 215 5

Poly(neopenthyl acrylate) 0.6 295 301 21 295 17 283 17

Poly(hexyl acrylate) 0.6 216 212 10 216 12 212 14

Poly(heptyl acrylate) 0.6 213 213 10 213 11 207 13

Poly(2-heptyl acrylate) 0.6 235 232 17 235 14 229 13

Poly(octyl acrylate) 0.6 208 205 11 208 14 207 15

Poly(2-octyl acrylate) 0.6 228 225 12 228 13 232 10

Poly(2-methylbutyl acrylate) 0.6 241 240 9 241 11 240 15

Poly(3-methylbutyl acrylate) 0.6 228 228 14 228 15 238 19

Poly(2-methylpentyl acrylate) 0.6 235 236 12 235 13 234 11

Poly(1,3-dimethylbutyl acrylate) 0.6 258 258 14 258 10 263 12

Poly(2-methyl-7-ethyl-4-undecyl acrylate) 0.6 253 240 21 253 11 257 13

Poly(3-thiabutyl acrylate) 0.6 213 216 10 213 18 213 9

Poly(3-thiapentyl acrylate) 0.6 202 211 12 202 9 209 13

Poly(4-thiahexyl acrylate) 0.6 197 206 15 197 10 206 14

Poly(5-thiahexyl acrylate) 0.6 203 203 8 203 10 206 10

Poly(fluoromethyl acrylate) 0.6 288 279 16 288 13 295 15

Poly(2,2,2-trifluoroethyl acrylate) 0.6 263 267 13 263 11 263 14

Poly(heptafluoro-2-propyl acrylate) 0.6 278 280 12 278 16 277 12

Poly(1H,1H-pentafluoropropyl acrylate) 0.6 247 243 14 247 15 249 13

Poly(3-chloro-2,2-bis(chloromethyl)propyl acrylate) 0.6 319 321 18 319 14 320 16

Poly(1H,1H-heptafluorobutyl acrylate) 0.6 243 242 9 243 10 248 11

Poly(1H,1H,3H-hexafluorobutyl acrylate) 0.6 251 259 15 251 14 257 15

Poly(1H,1H,5H-octafluoropentyl acrylate) 0.6 238 246 18 238 13 244 13

Poly(1H,1H-undecafluorohexyl acrylate) 0.6 234 235 13 234 9 230 10

Poly(2,2,3,3,5,5,5-heptafluoro-4-oxapentyl acrylate) 0.6 218 223 17 218 12 220 13

Table 2. continued.

Polymer Molar Tg Exp. 1 Exp. 2 Exp. 3

fraction (K) Out  Out  Out 

of *r* dyads (K) (K) (K) (K) (K) (K)

Poly(4,4,5,5-tetrafluoro-3-oxapentyl acrylate) 0.6 251 253 18 251 20 248 22

Poly(5,5,6,6,7,7,7-heptafluoro-3-oxaheptyl acrylate) 0.6 228 227 11 228 12 227 10

Poly(1H,1H-undecafluoro-4-oxaheptyl acrylate) 0.6 205 222 20 205 21 213 12

Poly(cyanomethyl acrylate) 0.6 433 388 47 433 44 395 42

Poly(2-cyanoethyl acrylate) 0.6 277 289 19 277 21 293 26

Poly(2-cyano*iso*propyl acrylate) 0.6 339 333 23 339 18 337 14

Poly(2-cyano*iso*butyl acrylate) 0.6 324 338 22 324 24 327 13

Poly(4-cyanobutyl acrylate) 0.6 233 238 13 233 20 237 12

Poly(2-cyanohexyl acrylate) 0.6 358 361 12 358 13 360 19

Poly(2-cyanoheptyl acrylate) 0.6 389 384 17 389 17 373 23

Poly(5-cyano-3-oxapentyl acrylate) 0.6 250 241 15 250 16 240 18

Poly(4-cyano-3-thiabutyl acrylate) 0.6 249 256 17 249 9 251 15

Poly(5-cyano-3-thiapentyl acrylate) 0.6 214 226 21 214 20 227 16

Poly(6-cyano-4-thiahexyl acrylate) 0.6 215 216 16 215 13 221 11

Poly(8-cyano-7-thiaoctyl acrylate) 0.6 223 221 9 223 18 230 12

Poly(2-methoxyethyl acrylate) 0.6 223 221 13 223 14 219 13

Poly(3-methoxypropyl acrylate) 0.6 198 213 25 198 17 205 12

Poly(3-ethoxypropyl acrylate) 0.6 218 213 10 218 11 214 9

Poly(3-methoxybutyl acrylate) 0.6 217 226 17 217 18 219 8

Poly(acrylamide) 0.6 438 440 14 438 14 440 17

Poly(N,N-dimethylacrylamide) 0.6 362 376 19 362 11 370 15

Poly(N-*iso*propylacrylamide) 0.6 358 373 23 358 15 363 13

Poly(N,N-di*iso*propylacrylamide) 0.6 393 390 8 393 13 378 18

Poly(N-butylacrylamide) 0.6 319 311 18 319 12 316 19

Poly(N-*ter*butylacrylamide) 0.6 401 389 23 401 14 400 8

Poly(N,N-dibutylacrylamide) 0.6 333 317 19 333 23 324 18

Poly(N-(1-methylbutyl)acrylamide) 0.6 380 352 33 380 22 373 19

Poly(N-octylacrylamide) 0.6 220 256 41 220 24 233 23

Poly(ethyl ethacrylate) 0.6 300 312 23 300 9 301 12

Poly[(1-methoxycarbonyl-1-methoxycarbonylmethylene) 0.6 372 371 10 372 13 367 12

ethylene]

Poly(ethyl ethoxycarbonylmethacrylate) 0.7 325 331 17 325 16 333 17

Poly(hexyl hexyloxycarbonylmethacrylate) 0.7 269 267 13 269 17 262 13

Poly(methyl fluoroacrylate) 0.6 404 407 9 404 7 401 8

Poly(methyl fluoromethacrylate) 0.6 357 368 19 357 15 365 13

Poly(ethyl fluoromethacrylate) 0.6 316 324 17 316 15 315 11

Table 2. continued.

Polymer Molar Tg Exp. 1 Exp. 2 Exp. 3

fraction (K) Out  Out  Out 

of *r* dyads (K) (K) (K) (K) (K) (K)

Poly(methyl chloroacrylate) 0 358 371 16 358 13 372 15

0.35 380 396 17 380 14 395 15

0.52 409 407 6 409 4 406 6

0.59 411 411 5 411 2 411 5

Poly(methyl chloroacrylate) 0.71 419 417 6 419 4 418 5

0.75 424 419 7 424 6 420 6

1 450 429 22 450 20 433 19

Poly(methyl b-chloroacrylate) 0.6 416 387 35 416 28 404 17

Poly(ethyl chloroacrylate) 1 404 379 26 404 23 383 22

0.8 377 370 8 377 7 372 7

0.71 367 366 4 367 5 367 5

0.54 356 356 4 356 5 356 4

0.27 325 337 13 325 11 337 12

0.16 320 328 10 320 9 329 10

0 308 317 11 308 11 319 13

Poly(propyl chloroacrylate) 0.6 344 346 14 344 12 344 11

Poly(*sec*butyl chloroacrylate) 0.6 347 348 16 347 12 353 14

Poly(butyl cyanoacrylate) 0.6 358 333 31 358 28 342 23

Poly(*iso*propyl chloroacrylate) 0 341 345 8 341 10 347 9

0.05 343 348 8 343 10 350 9

0.34 366 367 5 366 6 366 6

0.36 369 369 5 369 7 367 6

0.64 383 387 7 383 8 384 7

0.87 402 399 6 402 10 398 7

1 409 404 8 409 11 405 7

Poly(methacrylic acid) 0.7 501 483 25 501 14 495 14

Poly(methyl methacrylate) 0.01 328 333 10 328 13 332 11

0.64 367 374 8 367 9 374 9

0.74 378 378 4 378 6 379 5

0.79 382 380 4 382 5 382 5

0.83 388 382 7 388 6 384 7

0.96 396 387 10 396 8 390 10

0.99 403 388 15 403 12 391 14

Poly(propyl methacrylate) 0.7 308 305 15 308 20 306 10

Poly(*iso*propyl methacrylate) 0.75 359 355 11 359 15 350 12

0 307 312 12 307 13 307 8

Poly(butyl methacrylate) 0.7 293 287 12 293 11 286 13

Poly(butyl methacrylate) 0 249 250 11 249 9 248 9

Poly(*sec*butyl methacrylate) 0.7 333 319 16 333 22 317 19

Poly(*ter*butyl methacrylate) 0.75 391 378 17 391 14 382 13

0.55 359.5 369 13 360 15 372 15

0.1 350 343 13 350 10 342 10

Poly(pentyl methacrylate) 0.7 268 271 14 268 13 269 14

Poly(neopentyl methacrylate) 0.7 312 324 24 312 26 325 22

Table 2. continued.

Polymer Molar Tg Exp. 1 Exp. 2 Exp. 3

fraction (K) Out  Out  Out 

of *r* dyads (K) (K) (K) (K) (K) (K)

Poly(hexyl methacrylate) 0.7 268 270 15 268 14 274 13

Poly(dodecyl methacrylate) 0.7 208 232 28 208 29 230 29

Poly(2-ethylhexyl methacrylate) 0.7 263 271 15 263 11 266 11

Poly(3,3-dimethyl-2-butylbutyl methacrylate) 0.7 381 376 10 381 15 372 18

Poly(3,5,5-trimethylhexyl methacrylate) 0.7 274 274 11 274 19 286 21

Poly(dimethylaminoethyl methacrylate) 0.7 292 307 19 292 14 298 20

Poly(2-*ter*butylaminoethyl methacrylate) 0.7 306 318 17 306 21 313 15

Poly(2-chloroethyl methacrylate) 0.7 365 356 16 365 22 353 17

Poly(2-bromoethyl methacrylate) 0.7 325 327 10 325 12 330 17

Poly(1,1,1-trifluoro-2-propyl methacrylate) 0.7 354 349 13 354 16 345 17

Poly(1H,1H-heptafluorobutyl methacrylate) 1 330 317 19 330 20 320 14

Poly(1H,1H,5H-octafluoropentyl methacrylate) 0.7 309 301 16 309 27 295 20

Poly(1H,1H,9H-hexadecafluorononyl methacrylate) 0.7 258 273 21 258 18 267 17

Poly(2-cyanoethyl methacrylate) 0.7 364 359 15 364 17 357 15

Poly(3-oxa-butyl methacrylate) 0.7 289 284 16 289 9 283 14

o Poly(2-methoxyethyl methacrylate)

Poly(3-oxa-5-hydroxypentyl methacrylate) 0.7 278 281 16 278 13 289 17

Poly(2-hydroxyethyl methacrylate) 0.7 359 346 16 359 11 346 15

Poly(2-hydroxyethyl methacrylate) 0.2 311 315 13 311 11 318 12

Poly(2-ethylsulfinylethyl methacrylate) 0.7 298 285 15 298 17 291 14

Poly(2-nitratoethyl methacrylate) 0.7 328 330 13 328 14 331 13

Poly(2-ethylbutyl methacrylate) 0.7 284 289 12 284 13 286 12

Poly(phenyl acrylate) 0.79 323 335 18 323 14 333 12

0.56 333 323 17 333 13 319 17

Poly(2-phenylethyl acrylate) 0.6 270 284 22 270 22 281 23

Poly(2-methylphenyl acrylate) 0.6 325 327 15 325 11 326 8

Poly(3-methylphenyl acrylate) 0.6 298 302 11 298 23 324 28

Poly(4-methylphenyl acrylate) 0.6 316 337 24 316 13 320 8

Poly(2-*ter*butylphenyl acrylate) 0.6 345 344 10 345 17 342 16

Poly(4-*ter*butylphenyl acrylate) 0.6 344 339 14 344 15 342 16

Poly(2-chlorophenyl acrylate) 0.79 318 336 23 318 21 336 22

Poly(4-chlorophenyl acrylate) 0.79 330 339 15 330 11 338 13

Poly(2,4-dichlorophenyl acrylate) 0.6 333 327 12 333 12 327 13

Poly(3-dimethylaminophenyl acrylate) 0.6 320 313 12 320 24 327 17

Poly(4-cyanophenyl acrylate) 0.6 363 354 15 363 13 354 21

Poly(4-methoxyphenyl acrylate) 0.6 324 326 13 324 7 322 11

Table 2. continued.

Polymer Molar Tg Exp. 1 Exp. 2 Exp. 3

fraction (K) Out  Out  Out 

of *r* dyads (K) (K) (K) (K) (K) (K)

Poly[ethyl 2-(acryloyloxy)benzoate] 0.6 303 298 13 303 19 315 17

Poly[ethyl 3-(acryloyloxy)benzoate] 0.6 297 303 11 297 21 311 20

Poly[ethyl 4-(acryloyloxy)benzoate] 0.6 310 314 15 310 12 306 10

Poly[butyl 4-(acryloyloxy)benzoate] 0.6 286 289 13 286 19 301 19

Poly(N-methyl-N-phenylacrylamide) 0.7 453 435 22 453 34 420 39

Poly(benzyl methacrylate) 0.75 327 337 17 327 27 344 24

Poly(2-phenylethyl methacrylate) 0.75 299 322 28 299 34 323 29

Poly(4-*ter*butylphenyl methacrylate) 0.66 403 393 17 403 12 398 14

Poly[methyl 4-(methacryloyloxy)benzoate] 0.7 379 383 13 379 13 379 15

Poly(4-cyanophenyl methacrylate) 0.7 428 412 22 428 17 419 16

Poly[4-(cyanomethyl)phenyl methacrylate] 0.7 401 398 13 401 21 388 17

Poly[4-(methacrylamido)benzoic acid] 0.7 473 465 14 473 24 462 20

Poly[methyl 4-(methacrylamido)benzoate] 0.7 453 452 12 453 24 445 14

Poly[butyl 4-(methacrylamido)benzoate] 0.7 401 408 16 401 15 413 23

Poly(methyl atropate) 0.7 391 417 29 391 27 410 22

0 397 372 26 397 22 378 21

Poly(2-methylphenyl methacrylate) 0.76 382 383 11 382 14 379 13

Poly(3-methylphenyl methacrylate) 0.7 380 371 14 380 12 388 12

Poly(4-methylphenyl methacrylate) 0.7 403 394 17 403 24 386 19

Poly(2,3-dimethylphenyl 2-methylacrylate) 0.7 398 383 21 398 14 381 22

Poly(3,4-dimethylphenyl 2-methylacrylate) 0.7 384 388 11 384 12 383 9

Poly(biphenyl-4-yl 2-methylacrylate) 0.72 413 412 12 413 13 414 11

Poly(4-fluorophenyl acrylate) 0.52 325 320 12 325 8 319 10

Poly[6-((4’-methoxybiphenyl-4-yl)oxy)hexyl acrylate] 0.6 338 322 18 338 20 316 24

Poly[3-(4-(4-nitrophenyldiazenyl)phenoxy)propyl acrylate] 0.6 319 317 11 319 15 325 11

Poly[6-(4-(4-nitrophenyldiazenyl)phenoxy)hexyl acrylate] 0.6 309 315 12 309 11 313 9

Poly[2-((4’-cyanobiphenyl-4-yl)oxy)ethyl acrylate] 0.6 323 325 13 323 18 322 11

Poly[5-((4’-cyanobiphenyl-4-yl)oxy)pentyl acrylate] 0.6 313 312 19 313 16 309 16

Poly[11-((4’-cyanobiphenyl-4-yl)oxy)undecyl acrylate] 0.6 303 310 9 303 12 309 14

Poly[2-(2-(2-((4’-methoxybiphenyl-4-yl)oxy)ethoxy)- 0.6 344 323 25 344 27 327 22

ethoxy)ethyl acrylate]

Poly[6-(4-(4-cyanophenyldiazenyl)phenoxy)hexyl 0.6 300 311 16 300 15 310 13

acrylate]

Poly[4-(4-dimethylaminophenyldiazenyl)phenyl 0.6 392 388 21 392 27 364 33

acrylate]

Poly[11-(4-(4-dimethylaminophenyldiazenyl)- 0.6 321 313 11 321 15 313 14

phenoxy)undecyl acrylate]

Table 2. continued.

Polymer Molar Tg Exp. 1 Exp. 2 Exp. 3

fraction (K) Out  Out  Out 

of *r* dyads (K) (K) (K) (K) (K) (K)

Poly(biphenyl-2-yl acrylate) 0.6 378 363 22 378 30 352 30

Poly[2-(4-(4-pentyloxyphenyldiazenyl)-2-methyl- 0.6 294 292 20 294 21 308 16

phenoxy)hexyl acrylate]

Poly[6-(((4’-((S)-1-methylheptyl)oxy)biphenyl-4-yl)- 0.6 321 321 5 321 8 316 8

oxy)hexyl acrylate]

Poly[4’-((6-(acryloyloxy)hexyloxy)biphenyl-4-yl) 0.6 301 318 18 301 20 315 15

(2S,3S)-2-chloro-3-methylpentanoate]

Poly[11-((4’-((S)-2-methylbutoxy)biphenyl-4-yl)oxy) 0.6 328 316 15 328 19 313 19

undecyl acrylate]

Poly[4’-((11-(acryloyloxy)undecyloxy)- 0.6 318 312 10 318 11 312 12

biphenyl-4-yl) (S)-2-chloro-3-methylbutanoate]

Poly[4-(6-(acryloyloxy)hexyloxy)benzoic acid] 0.6 339 323 19 339 25 323 22

Poly(2-chlorophenyl methacrylate) 0.7 384 381 12 384 14 386 15

Poly(4-chlorophenyl methacrylate) 0.7 404 390 20 404 22 389 17

Poly[4-(3-methoxy-3-oxopropyl)phenyl methacrylate] 0.7 341 347 13 341 34 375 36

Poly[methyl 2-(methacryloyloxy)benzoate] 0.7 337 343 10 337 31 369 35

Poly[methyl 3-(methacryloyloxy)benzoate] 0.7 345 362 20 345 29 359 21

Poly[2-(methacryloyloxy)benzoic acid] 0.7 403 414 18 403 21 395 13

Poly[3-(methacryloyloxy)benzoic acid] 0.7 389 386 15 389 14 393 16

Poly[2-((4’-cyanobiphenyl-4-yl)oxy)ethyl methacrylate] 0.7 368 367 12 368 11 370 12

Poly[11-((4’-cyanobiphenyl-4-yl)oxy)undecyl 0.7 313 324 17 313 15 314 13

methacrylate]

Poly[11-(4’-cyanobiphenyl-4-yl)undecyl methacrylate] 0.7 303 321 22 303 13 309 11

Poly[11-((4’-cyanobiphenyl-4-yl)oxy)-11-oxoundecyl 0.7 318 318 12 318 11 315 13

methacrylate]

Poly[4’-methoxybiphenyl-4-yl 4-(6-(methacryloyloxy)- 0.7 333 338 10 333 15 344 15

hexyloxy)benzoate]

Poly[6-(methyl(4-((4-methylsulfonylphenyldiazenyl)- 0.7 373 355 24 373 18 360 18

phenyl)amino)hexyl methacrylate]

Poly[N-(2-methyl-4-(2-methylphenyldiazenyl) 0.7 436 440 13 436 20 449 20

phenyl)methacrylamide]

Poly[2-(((4-cyanophenyldiazenyl)phenyl)- 0.7 384 382 15 384 11 377 15

(2-methylbutyl)amino)ethyl acrylate]

Poly[2-(4-(phenyldiazenyl)phenoxy)ethyl methacrylate] 0.7 378 366 15 378 14 369 15

Poly[4-(4-(4-cyanophenyldiazenyl)phenoxy)butyl 0.7 353 344 16 353 16 350 18

methacrylate]

Poly[8-(4-(4-cyanophenyldiazenyl)phenoxy)octyl 0.7 308 322 16 308 19 318 13

methacrylate]

Poly[2-(2-(2-(2-((4-cyanophenyldiazenyl)phenoxy)- 0.7 293 312 25 293 21 299 17

ethoxy)ethoxy)ethoxy)ethyl methacrylate]

Table 2. continued.

Polymer Molar Tg Exp. 1 Exp. 2 Exp. 3

fraction (K) Out  Out  Out 

of *r* dyads (K) (K) (K) (K) (K) (K)

Poly[6-(4-(4-methoxyphenyldiazenyl)phenoxy)hexyl 0.7 341 342 9 341 11 344 9

methacrylate]

Poly[4-(4-dimethylaminophenyldiazenyl)phenyl 0.7 457 432 28 457 38 421 39

methacrylate]

Poly[6-(4-(4-dimethylaminophenyldiazenyl) 0.7 359 343 19 359 13 350 14

phenoxy)hexyl methacrylate]

Poly[2-(4-*ter*butylphenoxy)-2-oxoethyl methacrylate] 0.7 368 367 14 368 16 364 17

Poly(4-benzoylphenyl methacrylate) 0.7 391 408 22 391 21 401 21

Poly[2-(2-((4-cyanophenyldiazenyl)phenoxy)ethoxy)- 0.7 314 338 25 314 27 339 27

ethyl methacrylate]

Poly[4-((6-((2-mehtyl-1-oxo-2-propenyl)oxy)hexyl)oxy)- 0.7 357 339 20 357 14 347 15

benzoic acid 4’-((1-oxo-10,12-nonadecadiynyl)oxy)-

(1,1’-biphenyl)-4-yl)ester]