

## Holdout Test Results

Solvent	RMSE (kcal/mol)	Count	Dielectric Constant ( $\epsilon$ )
Bromooctane	$0.077 \pm 0.034$	5	5.0244
Fluorooctane	$0.084 \pm 0.009$	6	3.89
Pentadecane	$0.086 \pm 0.018$	9	2.0333
Isopropyltoluene	$0.089 \pm 0.021$	6	2.2322
Tbutylbenzene	$0.092 \pm 0.026$	14	2.3447
Trimethylbenzene	$0.096 \pm 0.015$	11	2.3653
Isopropylbenzene	$0.103 \pm 0.015$	19	2.3712
Mesitylene	$0.11 \pm 0.025$	7	2.265
Nonane	$0.134 \pm 0.004$	26	1.9605
Chlorohexane	$0.141 \pm 0.033$	11	5.9491
Butylbenzene	$0.162 \pm 0.022$	10	2.36
Secbutylbenzene	$0.168 \pm 0.011$	5	2.3446
Nitromethane	$0.171 \pm 0.052$	7	36.5623
Bromobenzene	$0.173 \pm 0.012$	27	5.3954
Chlorobenzene	$0.175 \pm 0.017$	38	5.6968
Heptanol	$0.185 \pm 0.025$	12	11.321
Pentane	$0.19 \pm 0.009$	26	1.8371
Hexadecyl iodide	$0.19 \pm 0.041$	9	3.5338
Anisole	$0.192 \pm 0.042$	8	4.2247
Ethylbenzene	$0.198 \pm 0.007$	29	2.4339
Benzonitrile	$0.203 \pm 0.076$	7	25.592
Dibromoethane	$0.205 \pm 0.033$	10	4.9313
Ethoxybenzene	$0.21 \pm 0.035$	7	4.1797
Octane	$0.211 \pm 0.022$	38	1.9406
Onitrotoluene	$0.213 \pm 0.098$	6	25.6692
Fluorobenzene	$0.213 \pm 0.112$	7	5.42

Dodecane	$0.227 \pm 0.017$	8	2.006
Pyridine	$0.232 \pm 0.057$	7	12.9776
Bromoform	$0.232 \pm 0.046$	12	4.2488
Decane	$0.232 \pm 0.014$	39	1.9846
Nonanol	$0.242 \pm 0.064$	10	8.5991
Nitroethane	$0.249 \pm 0.118$	7	28.2896
Undecane	$0.252 \pm 0.035$	13	1.991
Dibutylether	$0.253 \pm 0.105$	15	3.0473
Methylenechloride	$0.266 \pm 0.03$	11	8.93
Iodobenzene	$0.269 \pm 0.012$	20	4.547
2-Methylpyridine	$0.278 \pm 0.111$	6	9.9533
Nitrobenzene	$0.279 \pm 0.036$	15	34.8091
Dimethylformamide	$0.285 \pm 0.051$	7	37.219
o-Dichlorobenzene	$0.296 \pm 0.025$	11	9.9949
Butanol	$0.3 \pm 0.033$	21	17.3323
Xylene	$0.302 \pm 0.026$	48	2.3879
Decanol	$0.312 \pm 0.024$	11	7.5305
Toluene	$0.314 \pm 0.006$	51	2.3741
Hexanol	$0.32 \pm 0.046$	14	12.5102
Isooctane	$0.329 \pm 0.029$	32	1.9358
Perfluorobenzene	$0.338 \pm 0.14$	15	2.029
Propanol	$0.339 \pm 0.093$	7	20.5237
Methylformamide	$0.292 \pm 0.10$	7	181.5619
Benzylalcohol	$0.365 \pm 0.011$	10	12.4569
Hexane	$0.369 \pm 0.028$	59	1.8819
Acetophenone	$0.378 \pm 0.167$	9	17.44
Dichloroethane	$0.383 \pm 0.069$	39	10.125
Methoxyethanol	$0.385 \pm 0.066$	6	17.2

Heptane	$0.388 \pm 0.023$	69	1.9113
Phenylether	$0.391 \pm 0.115$	6	3.73
Trimethylamine	$0.4 \pm 0.039$	7	2.3832
Dimethylpyridine	$0.412 \pm 0.056$	6	7.1735
4-Methyl-2-pentanone	$0.42 \pm 0.052$	13	12.8871
carbontet	$0.423 \pm 0.067$	79	2.228
Butylacetate	$0.423 \pm 0.077$	22	4.9941
Tetrahydrofuran	$0.43 \pm 0.071$	7	7.4257
Diisopropylether	$0.435 \pm 0.071$	22	3.38
Pentanol	$0.436 \pm 0.036$	22	15.13
Benzene	$0.441 \pm 0.018$	75	2.2706
Isopropanol	$0.449 \pm 0.12$	7	19.2645
Dimethylacetamide	$0.452 \pm 0.082$	7	37.7807
Isobutanol	$0.462 \pm 0.081$	17	16.7766
Decalin	$0.467 \pm 0.024$	27	2.196
Ethylacetate	$0.472 \pm 0.048$	24	5.9867
Tetrachloroethene	$0.491 \pm 0.076$	10	2.268
Butanone	$0.524 \pm 0.039$	13	18.2457
Diethylether	$0.545 \pm 0.063$	72	4.24
Tetralin	$0.561 \pm 0.113$	9	2.771
Aceticacid	$0.564 \pm 0.05$	7	6.2528
Hexadecane	$0.58 \pm 0.023$	198	2.0402
Acetonitrile	$0.581 \pm 0.16$	7	35.6881
Secbutanol	$0.587 \pm 0.267$	9	15.9436
Tributylphosphate	$0.617 \pm 0.102$	16	8.1781
Cyclohexane	$0.642 \pm 0.072$	92	2.0165
Aniline	$0.642 \pm 0.19$	10	6.8882
Ethanol	$0.689 \pm 0.142$	8	24.852

Bromoethane	$0.713 \pm 0.228$	7	9.01
Cyclohexanone	$0.804 \pm 0.157$	10	15.6186
Chloroform	$0.828 \pm 0.036$	109	4.7113
Octanol	$0.85 \pm 0.052$	247	9.8629
m-Cresol	$0.863 \pm 0.045$	7	12.44
Carbondisulfide	$0.938 \pm 0.17$	15	2.6105
Tetrahydrothiophenedioxide	$1.004 \pm 0.06$	7	43.9622
dimethylsulfoxide	$1.358 \pm 0.064$	7	46.826
Water	$3.465 \pm 0.19$	390	78.36