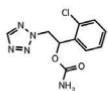


## SOLUBILITY PREDICTION

## SOLVENT SCREENING

Solute  
 NC(=O)OC(Cn1nc1) 



Solvent Set

custom

Solvents

O  
CO  
CCO  
CC(C)O  
CC(=O)O  
CC#N

Temperatures

298  
323

 Click to save  
custom solvent set

SUBMIT

... MORE OPTIONS

SAVE CUSTOM SOLVENT SET

CLEAR RESULTS

MODEL I/O DETAILS

Calculation Method

Method 1

Units

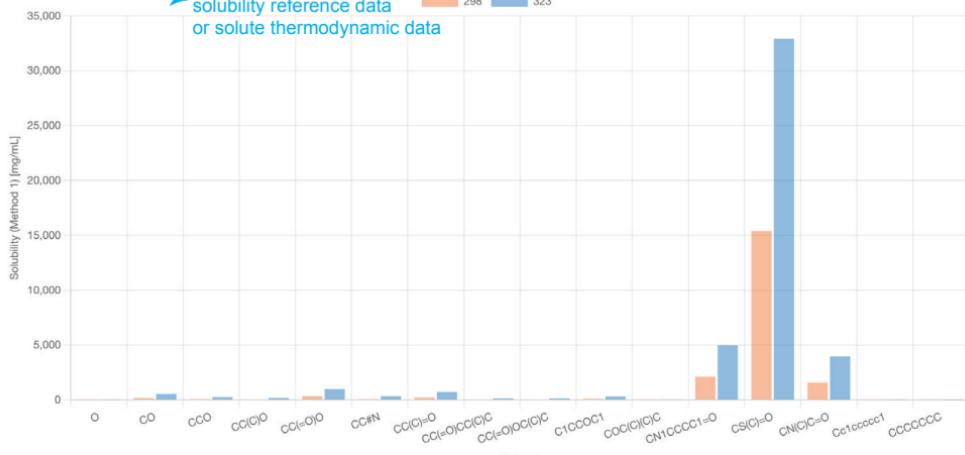
mg/mL

X Axis

solvent

DOWNLOAD

 Click to add  
solubility reference data or solute thermodynamic data  298  323



Solvent	SMILES	Solubility @ 298K (Method 1) [mg/mL]	Solubility @ 323K (Method 1) [mg/mL]
H <sub>2</sub> O	O	2.68	9.5