Chosen Data Set

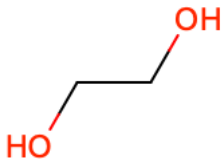
https://github.com/openforcefield/nistdataselection

A total of 43 data points covering 15 unique molecules are to be optimized against. This will require approximately 30 unique simulation to be performed.

SMIRKS	Pure Density	Pure Dielectric Constant	Pure Enthalpy Of Vaporization
'[#53X0-1:1]'	×	×	×
'[#8X2H1+0:1]'	✓	✓	✓
'[#17:1]'	✓	×	✓
'[#1:1]-[#7]'	✓	✓	✓
'[#1:1]-[#6X4] [*+1,*+2]'	×	×	×
'[#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]'	✓	✓	✓
'[#15:1]'	✓	×	✓
'[#6:1]'	✓	✓	✓
'[#35:1]'	✓	×	✓
'[#3+1:1]'	×	×	×
'[#1:1]-[#8]'	✓	✓	✓
'[#55+1:1]'	×	×	×
'[#1:1]-[#6X4]'	✓	✓	✓
'[#37+1:1]'	×	×	×
'[#19+1:1]'	×	×	×
'[#1:1]-[#6X2]'	×	×	×
'[#7:1]'	✓	✓	✓
'[#1:1]'	×	×	×
'[#1:1]-[#6X4](-[#7,#8,#9,#16,#17,#35])(-[#7,#8,#9,#16,#17,#35])-[#7,#8,#9,#16,#17,#35]'	×	×	×
'[#1:1]-[#6X4](-[#7,#8,#9,#16,#17,#35])-[#7,#8,#9,#16,#17,#35]'	×	×	✓
'[#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]'	✓	✓	✓
'[#53:1]'	×	×	✓
'[#1:1]-[#6X3]([#7,#8,#9,#16,#17,#35]) [#7,#8,#9,#16,#17,#35]'	✓	✓	✓
'[#6X4:1]'	✓	✓	✓
'[#6X2:1]'	✓	✓	✓
'[#1:1]-[#6X3]'	✓	✓	✓
'[#9X0-1:1]'	×	×	×
'[#16:1]'	✓	✓	✓
'[#9:1]'	✓	×	✓
'[#35X0-1:1]'	×	×	×
'[#1:1]-[#16]'	×	×	×
'[#8X2H0+0:1]'	✓	✓	✓
'[#8:1]'	✓	✓	✓
'[#17X0-1:1]'	×	×	×
'[#11+1:1]'	×	×	×

C(CO)O

Structure



SMIRKS Exercised

- [#1:1]-[#8]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#8X2H1+0:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	j.jct.2012.08.024.xml
303.15	101.325	j.jct.2012.08.024.xml
318.15	101.325	j.jct.2012.08.024.xml

Pure Dielectric Constant Data

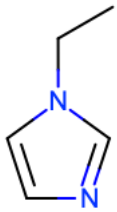
Temperature (K)	Pressure (kPa)	Source
303.15	101.325	j.fluid.2009.07.009.xml

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	je060333x.xml

CCn1ccnc1

Structure



SMIRKS Exercised

- [#7:1]
- [#6:1]
- [#1:1]-[#6X3]([#7,#8,#9,#16,#17,#35]) [#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X4]
- [#6X4:1]

Pure Density Data

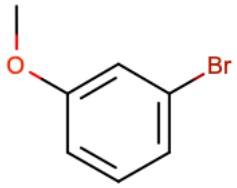
Temperature (K)	Pressure (kPa)	Source
298.15	101.325	j.fluid.2009.02.011.xml
318.15	101.325	j.fluid.2009.02.011.xml

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	j.jct.2014.08.020.xml

COc1cccc(c1)Br

Structure



SMIRKS Exercised

- [#6:1]
- [#35:1]
- [#8X2H0+0:1]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#1:1]-[#6X3]

Pure Density Data

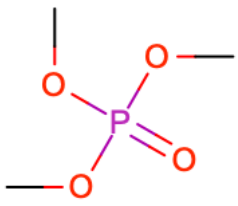
Temperature (K)	Pressure (kPa)	Source
303.15	101.325	acs.jced.5b00256.xml

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	j.jct.2008.11.008.xml

COP(=O)(OC)OC

Structure



SMIRKS Exercised

- [#15:1]
- [#8X2H0+0:1]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#8:1]
- [#6X4:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	j.fluid.2009.02.011.xml
318.15	101.325	j.fluid.2009.02.011.xml

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	j.tca.2007.10.007.xml

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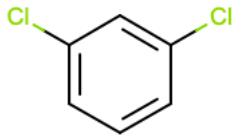
c1cc(cc(c1)Cl)Cl

Structure



SMIRKS Exercised

- [#6:1]
- [#17:1]
- [#1:1]-[#6X3]

Pure Density Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	j.jct.2013.12.024.xml
318.15	101.325	je600573w.xml

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	je5008795.xml

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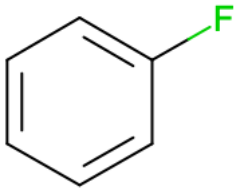
c1ccc(cc1)F

Structure



SMIRKS Exercised

- [#6:1]
- [#9:1]
- [#1:1]-[#6X3]

Pure Density Data

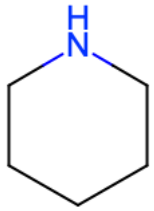
Temperature (K)	Pressure (kPa)	Source
293.2	101.325	je050231r.xml

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Source
293.2	101.325	j.fluid.2014.07.029.xml

C1CCNCC1

Structure



SMIRKS Exercised

- [#7:1]
- [#1:1]-[#7]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X4]
- [#6X4:1]

Pure Density Data

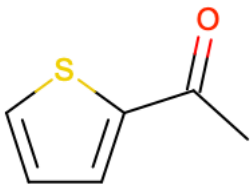
Temperature (K)	Pressure (kPa)	Source
298.15	101.325	j.jct.2007.05.009.xml
317.65	101.325	j.jct.2007.05.009.xml

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	j.jct.2013.08.005.xml

CC(=O)c1cccs1

Structure



SMIRKS Exercised

- [#6:1]
- [#16:1]
- [#8:1]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X4]
- [#6X4:1]
- [#1:1]-[#6X3]

Pure Density Data

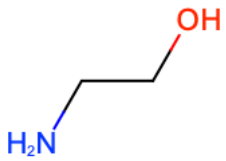
Temperature (K)	Pressure (kPa)	Source
298.15	101	j.fluid.2016.10.026.xml
318.15	101	j.fluid.2016.10.026.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Source
298.15	101	j.fluid.2016.10.026.xml
318.15	101	j.fluid.2016.10.026.xml

C(CO)N

Structure



SMIRKS Exercised

- [#7:1]
- [#8X2H1+0:1]
- [#1:1]-[#7]
- [#1:1]-[#8]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]

Pure Density Data

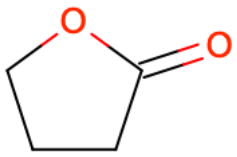
Temperature (K)	Pressure (kPa)	Source
303.15	101	je3013205.xml
318.15	101.325	j.fluid.2015.06.041.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Source
303.15	101	j.fluid.2008.01.024.xml

C1CC(=O)OC1

Structure



SMIRKS Exercised

- [#6:1]
- [#8:1]
- [#8X2H0+0:1]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X4]
- [#6X4:1]

Pure Density Data

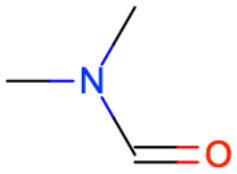
Temperature (K)	Pressure (kPa)	Source
298.15	101	je100803e.xml
313.15	101	je900503p.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Source
298.15	101	je900503p.xml
313.15	101	je900503p.xml

CN(C)C=O

Structure



SMIRKS Exercised

- [#7:1]
- [#6:1]
- [#8:1]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]([#7,#8,#9,#16,#17,#35]) [#7,#8,#9,#16,#17,#35]
- [#6X4:1]

Pure Density Data

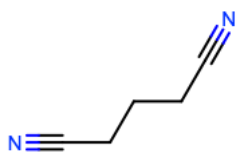
Temperature (K)	Pressure (kPa)	Source
303.15	101.325	je5002945.xml
318.15	101.325	j.jct.2012.04.007.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Source
318.12	101	je9010773.xml
303.15	101.325	j.fluid.2009.07.009.xml

C(CC#N)CC#N

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#6X4:1]
- [#6X2:1]
- [#7:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Source
298.15	101	acs.jced.6b00718.xml
313.15	101	acs.jced.6b00718.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	je300958c.xml
318.15	101.325	je300958c.xml

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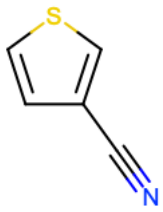
c1cscc1C#N

Structure



SMIRKS Exercised

- [#7:1]
- [#6:1]
- [#16:1]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6X2:1]
- [#1:1]-[#6X3]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	j.jct.2007.06.020.xml

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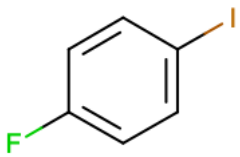
c1cc(ccc1F)I

Structure



SMIRKS Exercised

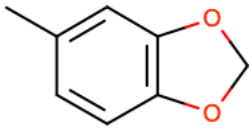
- [#6:1]
- [#53:1]
- [#9:1]
- [#1:1]-[#6X3]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	j.fluid.2014.12.023.xml

Cc1ccc2c(c1)OCO2

Structure



SMIRKS Exercised

- [#6:1]
- [#1:1]-[#6X4](-[#7,#8,#9,#16,#17,#35])-[#7,#8,#9,#16,#17,#35]
- [#8X2H0+0:1]
- [#1:1]-[#6X4]
- [#6X4:1]
- [#1:1]-[#6X3]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Source
298.15	101.325	je700035m.xml