Chosen Data Set https://github.com/openforcefield/nistdataselection

A total of 221 data points covering 104 unique molecules are to be optimized against. This will require approximately 242 unique simulation to be performed.

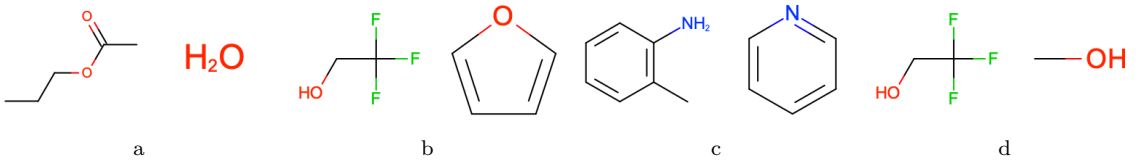
Data Points Per VdW SMIRKS Pattern

VdW SMIRKS	Binary H_{mix}	Binary V_{excess}	Pure ρ	Pure ΔH_{vap}	Pure ϵ_0
[#6X4:1]	49	32	66	26	30
[#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]	40	28	49	16	26
[#1:1]-[#6X4]	36	24	38	20	18
[#8:1]	35	24	18	16	8
[#1:1]-[#8]	35	16	29	6	22
[#6:1]	26	20	34	27	6
[#8X2H1+0:1]	24	14	29	6	22
[#8X2H0+0:1]	16	8	15	15	5
[#7:1]	15	6	19	7	8
[#1:1]-[#6X3]	11	6	17	26	1
[#9:1]	10	2	8	3	0
[#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]	9	6	11	14	1
[#35:1]	4	6	9	1	0
[#17:1]	4	4	10	2	0
[#16:1]	4	4	5	9	3

Unique Substances Per Data Type

Binary H_{mix}	Binary V_{excess}	Pure ρ	Pure ΔH_{vap}	Pure ϵ_0
29	16	77	30	30

Binary H_{mix}



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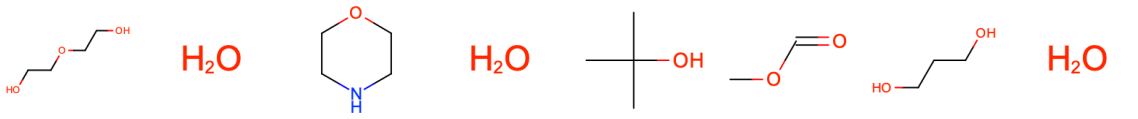

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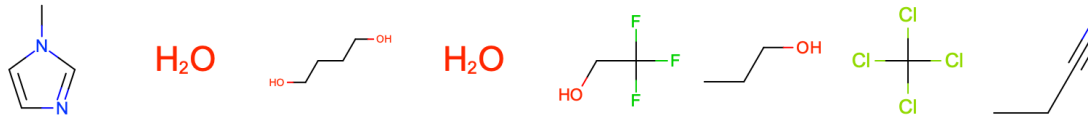

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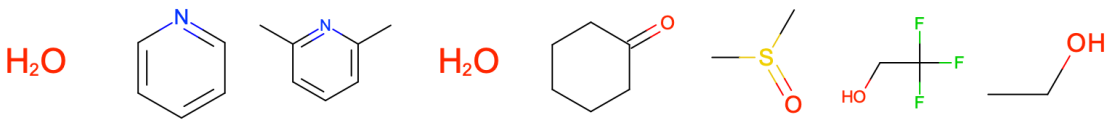

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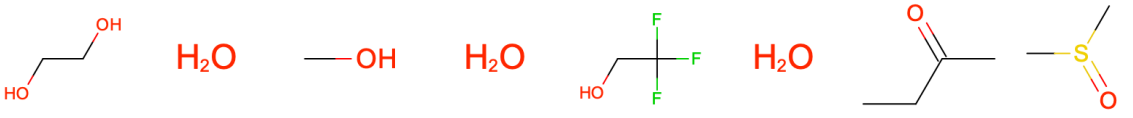

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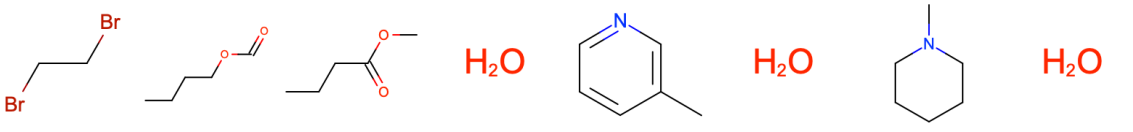

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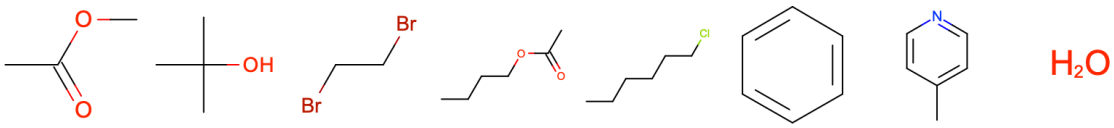

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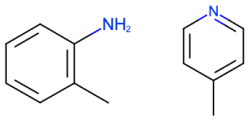

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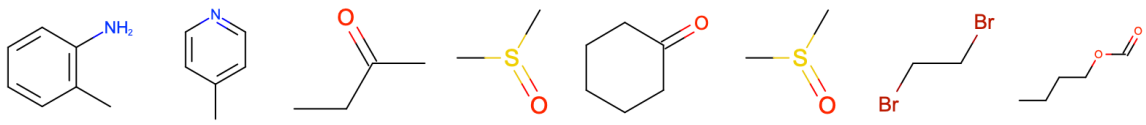
Binary V_{excess}



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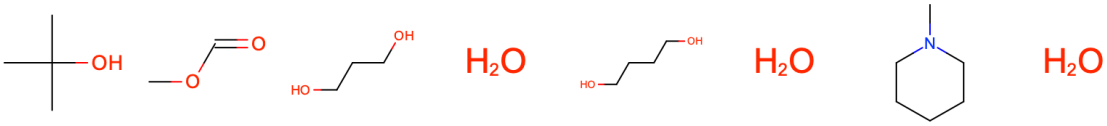

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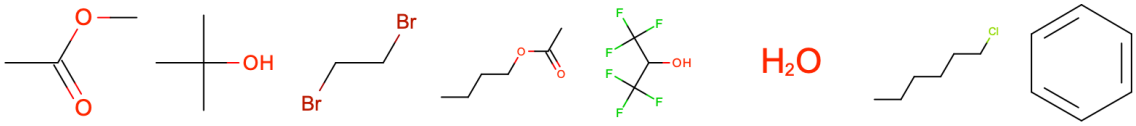

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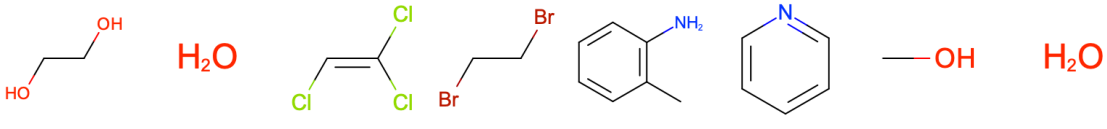

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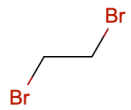
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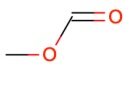
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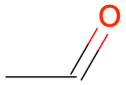
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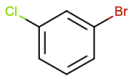
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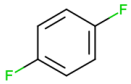
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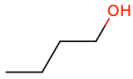
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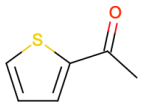
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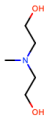
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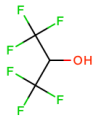
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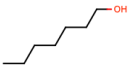
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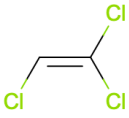
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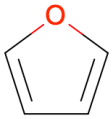
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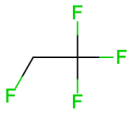
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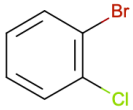
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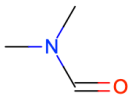
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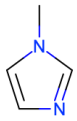
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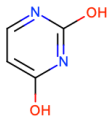
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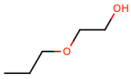
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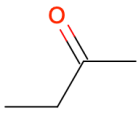
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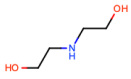
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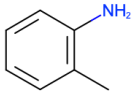
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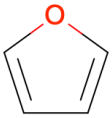
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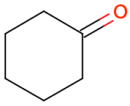
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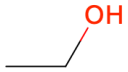
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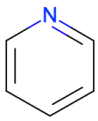
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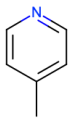
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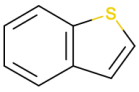
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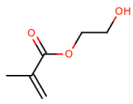
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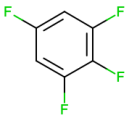
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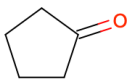
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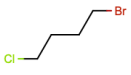
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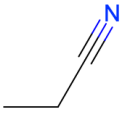
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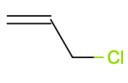
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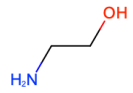
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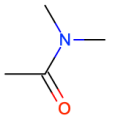
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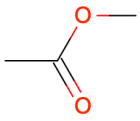
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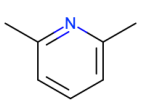
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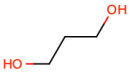
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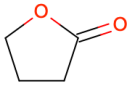
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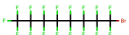
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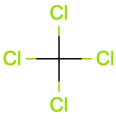
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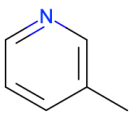
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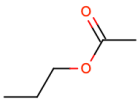
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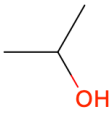
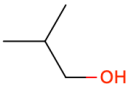
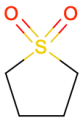

cy


cz


da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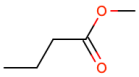
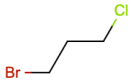
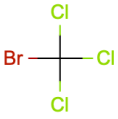
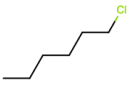

dc


dd


de


df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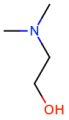
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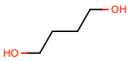
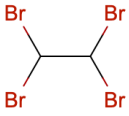
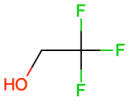
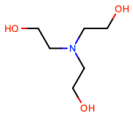

di


dj


dk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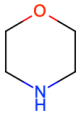
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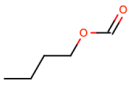
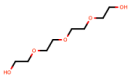
dn


do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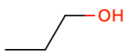
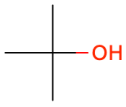
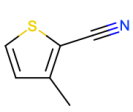
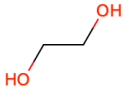

dq


dr

Pure ΔH_{vap}


ds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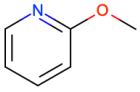
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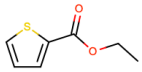
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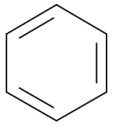
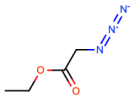
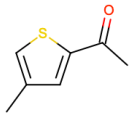

dw


dx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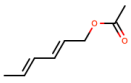
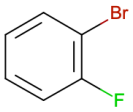

dz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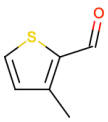
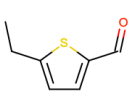

eb


ec

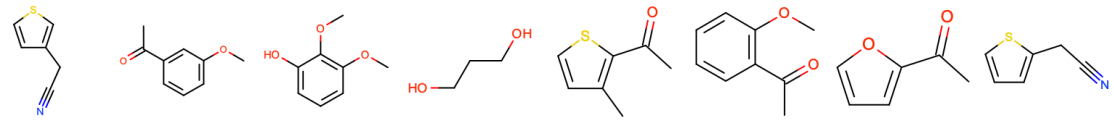
ed

ee

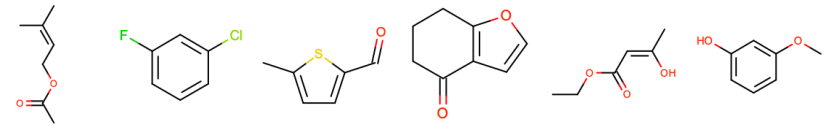
ef

eg

eh

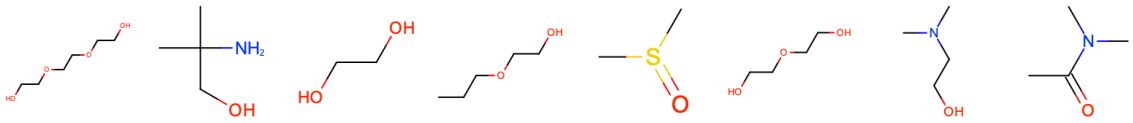


ei ej ek el em en eo ep

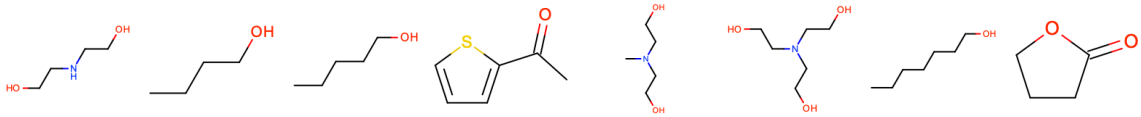


eq er es et eu ev

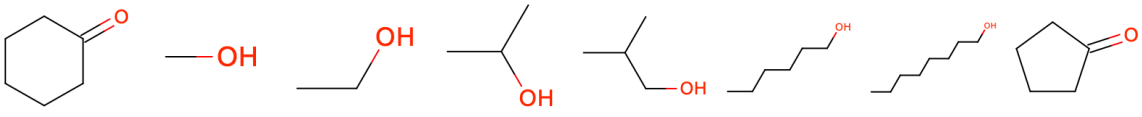
Pure ϵ_0



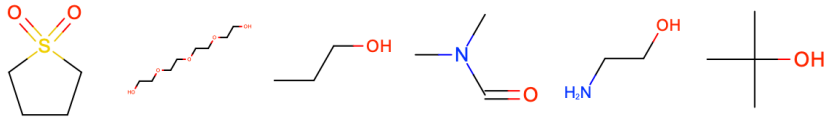
ew ex ey ez fa fb fc fd



fe ff fg fh fi fj fk fl



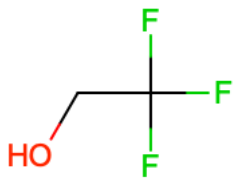
fm fn fo fp fq fr fs ft



fu fv fw fx fy fz

C(C(F)(F)F)O + C1CCOC1

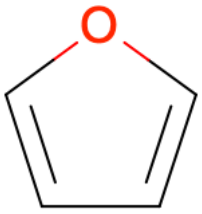
Structure



SMIRKS Exercised

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

Structure



SMIRKS Exercised

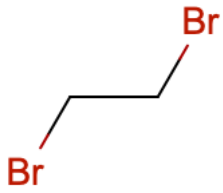
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#8X2H0+0:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101.3	0.212	0.788	je034076x.xml
298.15	101.3	0.717	0.283	je034076x.xml

C(CBr)Br

Structure



SMIRKS Exercised

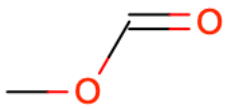
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#35:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
295.15	101.325	1	j.jct.2005.07.009.xml

COC=O

Structure



SMIRKS Exercised

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

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.fluid.2015.05.031.xml

CC=O

Structure

SMIRKS Exercised

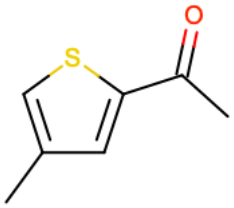
- [#1:1]-[#6X4]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
289.15	101.325	1	je300810p.xml

Cc1cc(sc1)C(=O)C

Structure



SMIRKS Exercised

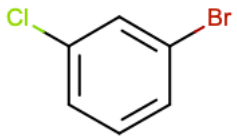
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#16:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2008.03.008.xml

c1cc(cc(c1)Br)Cl

Structure



SMIRKS Exercised

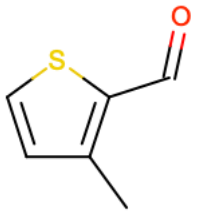
- [#1:1]-[#6X3]
- [#6:1]
- [#17:1]
- [#35:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je600573w.xml

Cc1ccsc1C=O

Structure



SMIRKS Exercised

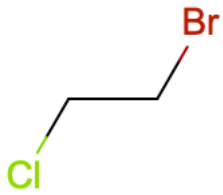
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#16:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2008.02.004.xml

C(CBr)Cl

Structure



SMIRKS Exercised

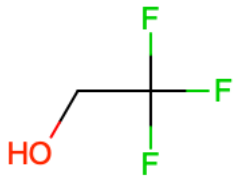
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#17:1]
- [#35:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je034259j.xml

C(C(F)(F)F)O + CCCO

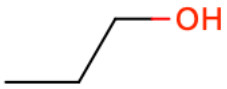
Structure



SMIRKS Exercised

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

Structure



SMIRKS Exercised

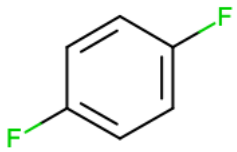
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H1+0:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.20133	0.79867	j.tca.2007.04.012.xml
298.15	101	0.79867	0.20133	j.tca.2007.04.012.xml

c1cc(ccc1F)F

Structure



SMIRKS Exercised

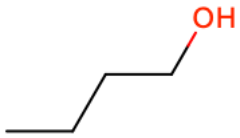
- [#1:1]-[#6X3]
- [#6:1]
- [#9:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
296.1	101.325	1	je8006474.xml

CCCCO

Structure



SMIRKS Exercised

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

Pure Density Data

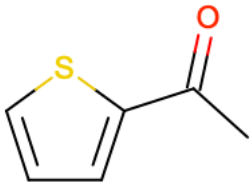
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	je300632p.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	je900503p.xml

CC(=O)c1cccs1

Structure



SMIRKS Exercised

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

Pure Density Data

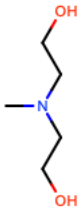
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	j.fluid.2016.10.026.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	j.fluid.2016.10.026.xml

CN(CCO)CCO

Structure



SMIRKS Exercised

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

Pure Density Data

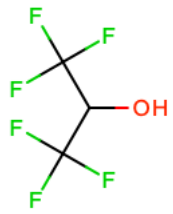
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	je050463q.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	je600515j.xml

C(C(F)(F)F)(C(F)(F)F)O

Structure



SMIRKS Exercised

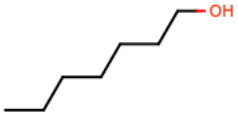
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H1+0:1]
- [#9:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je500455u.xml

CCCCCCCO

Structure



SMIRKS Exercised

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

Pure Density Data

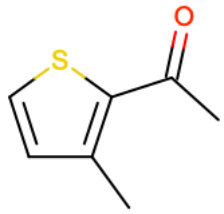
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	100	1	je500381c.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	100	1	je060248p.xml

Cc1ccsc1C(=O)C

Structure



SMIRKS Exercised

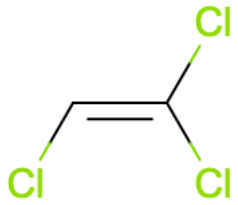
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#16:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2008.03.008.xml

$$C(=C(Cl)Cl)Cl$$

Structure



SMIRKS Exercised

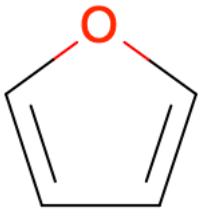
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#17:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je201211f.xml

c1ccoc1

Structure



SMIRKS Exercised

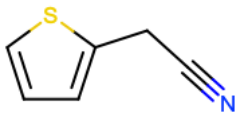
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#8X2H0+0:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
293.15	101.325	1	j.jct.2016.07.010.xml

c1cc(sc1)CC#N

Structure



SMIRKS Exercised

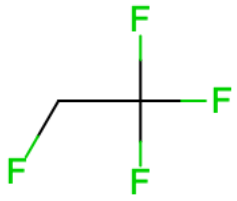
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X2:1]
- [#6X4:1]
- [#7:1]
- [#16:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2007.06.020.xml

C(C(F)(F)F)F

Structure



SMIRKS Exercised

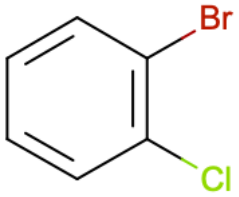
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#9:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
293.219	100.049	1	je0497496.xml

c1ccc(c(c1)Cl)Br

Structure



SMIRKS Exercised

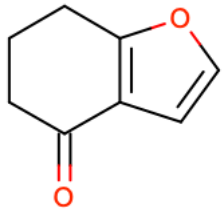
- [#1:1]-[#6X3]
- [#6:1]
- [#17:1]
- [#35:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je600573w.xml

c1coc2c1C(=O)CCC2

Structure



SMIRKS Exercised

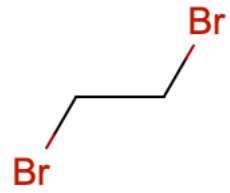
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2012.07.008.xml

C(CBr)Br + CCCCOC(=O)C

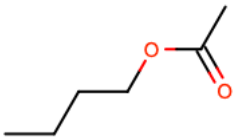
Structure



SMIRKS Exercised

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

Structure



SMIRKS Exercised

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

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2146	0.7854	j.jct.2009.05.006.xml
298.15	101	0.7661	0.2339	j.jct.2009.05.006.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2547	0.7453	j.jct.2009.05.006.xml
298.15	101	0.7476	0.2524	j.jct.2009.05.006.xml

C(=O)(C(F)(F)F)O

Structure

SMIRKS Exercised

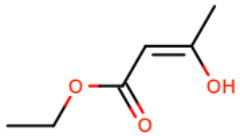
- [#1:1]-[#8]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H1+0:1]
- [#9:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
293.15	101.325	1	j.fluid.2015.08.012.xml

CCOC(=O)/C=C(/C)
O

Structure



SMIRKS Exercised

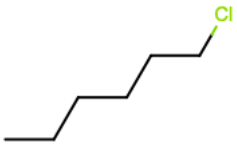
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#1:1]-[#8]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]
- [#8X2H1+0:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je050179z.xml

CCCCCCCl + c1ccccc1

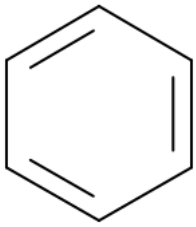
Structure



SMIRKS Exercised

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

Structure



SMIRKS Exercised

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

Binary Enthalpy Of Mixing Data

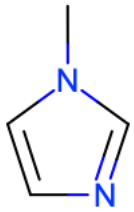
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2862	0.7138	je025625m.xml
298.15	101	0.7352	0.2648	je025625m.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2877	0.7123	je025625m.xml
298.15	101	0.772	0.228	je025625m.xml

Cn1ccnc1

Structure



SMIRKS Exercised

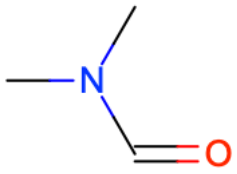
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]([#7,#8,#9,#16,#17,#35]) [#7,#8, #9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#7:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je200093f.xml

CN(C)C=O

Structure



SMIRKS Exercised

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

Pure Density Data

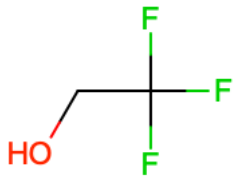
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	je5002945.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	j.fluid.2009.07.009.xml

C(C(F)(F)F)O + CO

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

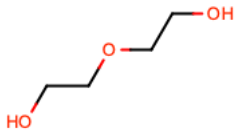
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H1+0:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.29705	0.70295	j.tca.2007.04.012.xml
298.15	101	0.70985	0.29015	j.tca.2007.04.012.xml

C(COCCO)O + O

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H0+0:1]
- [#8X2H1+0:1]

Structure

SMIRKS Exercised

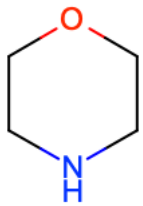
- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2002	0.7998	j.tca.2009.06.004.xml
298.15	101	0.7906	0.2094	j.tca.2009.06.004.xml

C1COCCN1 + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

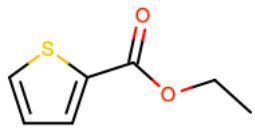
- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.7149	0.2851	j.jct.2015.06.006.xml
313.15	101	0.2968	0.7032	j.jct.2015.06.006.xml

CCOC(=O)c1cccs1

Structure



SMIRKS Exercised

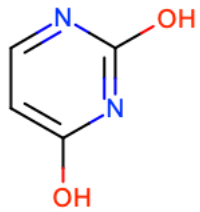
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]
- [#16:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2012.09.007.xml

c1cnc(nc1O)O

Structure



SMIRKS Exercised

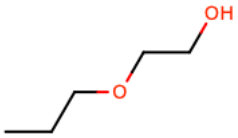
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#1:1]-[#8]
- [#6:1]
- [#8X2H1+0:1]
- [#7:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	j.jct.2012.07.022.xml

CCCOCCO

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H0+0:1]
- [#8X2H1+0:1]

Pure Density Data

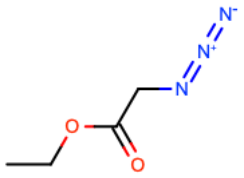
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	j.jct.2007.09.004.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	j.jct.2007.09.004.xml

CCOC(=O)CN=[N+]=[N-]

Structure



SMIRKS Exercised

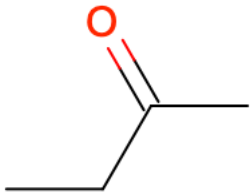
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]
- [#7:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2011.05.028.xml

CCC(=O)C

Structure



SMIRKS Exercised

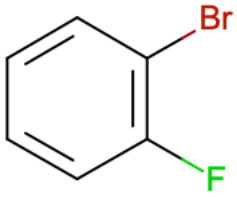
- [#1:1]-[#6X4]
- [#6:1]
- [#6X4:1]
- [#8:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.fluid.2015.04.017.xml

c1ccc(c(c1)F)Br

Structure



SMIRKS Exercised

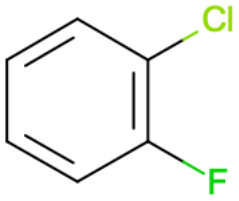
- [#1:1]-[#6X3]
- [#6:1]
- [#9:1]
- [#35:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.fluid.2014.12.023.xml

c1ccc(c(c1)F)Cl

Structure



SMIRKS Exercised

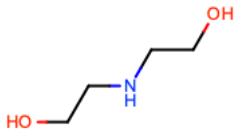
- [#1:1]-[#6X3]
- [#6:1]
- [#9:1]
- [#17:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.fluid.2014.12.023.xml

C(CO)NCCO

Structure



SMIRKS Exercised

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

Pure Density Data

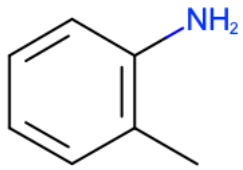
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	je050463q.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	je600515j.xml

Cc1ccccc1N

Structure



SMIRKS Exercised

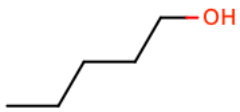
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#7]
- [#6:1]
- [#6X4:1]
- [#7:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2011.10.002.xml

CCCCCO

Structure



SMIRKS Exercised

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

Pure Density Data

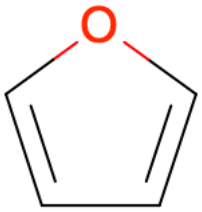
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.fluid.2015.03.040.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.tca.2012.05.036.xml

C1CCOC1

Structure



SMIRKS Exercised

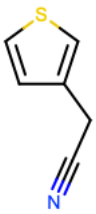
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#8X2H0+0:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2010.08.006.xml

c1cscc1CC#N

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X2:1]
- [#6X4:1]
- [#7:1]
- [#16:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2007.06.020.xml

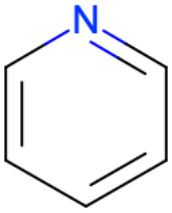
O + c1ccncc1

Structure

SMIRKS Exercised

- [#1:1]-[#8]
- [#8:1]

Structure



SMIRKS Exercised

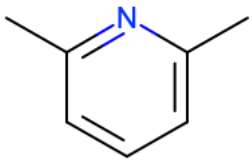
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#7:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
297.15	101	0.27	0.73	j.fluid.2009.10.018.xml
297.15	101	0.75	0.25	j.fluid.2009.10.018.xml

Cc1cccc(n1)C + O

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#6:1]
- [#6X4:1]
- [#7:1]

Structure

SMIRKS Exercised

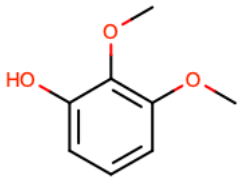
- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.004618	0.995382	je200093f.xml

COc1cccc(c1OC)O

Structure



SMIRKS Exercised

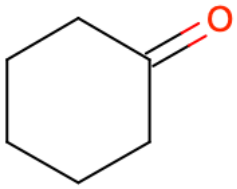
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#1:1]-[#8]
- [#6:1]
- [#6X4:1]
- [#8X2H0+0:1]
- [#8X2H1+0:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je025641j.xml

C1CCC(=O)CC1

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#6:1]
- [#6X4:1]
- [#8:1]

Pure Density Data

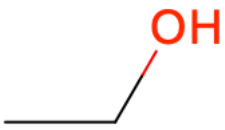
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2004.07.010.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je200682t.xml

CCO

Structure



SMIRKS Exercised

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

Pure Density Data

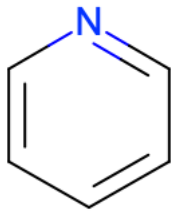
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	je1013476.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	j.fluid.2009.07.009.xml

c1ccncc1

Structure



SMIRKS Exercised

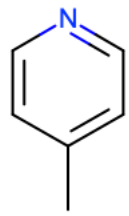
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#7:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je100472t.xml

Cc1ccncc1

Structure



SMIRKS Exercised

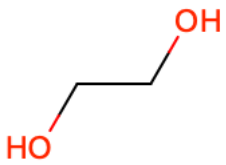
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#7:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2011.10.002.xml

C(CO)O + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

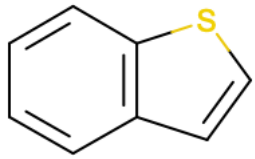
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2051	0.7949	j.tca.2009.06.004.xml
298.15	101	0.7909	0.2091	j.tca.2009.06.004.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.25008	0.74992	j.fluid.2013.06.041.xml
298.15	101	0.77876	0.22124	j.fluid.2013.06.041.xml

c1ccc2c(c1)ccs2

Structure



SMIRKS Exercised

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

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2013.12.029.xml

CC(=CCOC(=O)C)C

Structure

SMIRKS Exercised

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

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2015.02.015.xml

CO + O

Structure

SMIRKS Exercised

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

Structure

SMIRKS Exercised

- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

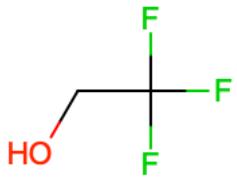
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2	0.8	j.tca.2006.02.028.xml
298.15	101	0.8	0.2	j.tca.2006.02.028.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	100	0.25	0.75	j.jct.2004.03.011.xml
298.15	100	0.75	0.25	j.jct.2004.03.011.xml

C(C(F)(F)F)O + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

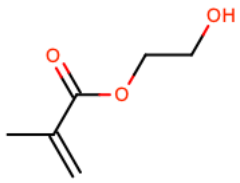
- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.29878	0.70122	j.tca.2007.04.012.xml
298.15	101	0.70779	0.29221	j.tca.2007.04.012.xml

CC(=C)C(=O)OCCO

Structure



SMIRKS Exercised

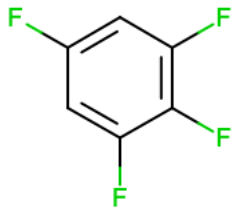
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#1:1]-[#8]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]
- [#8X2H1+0:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je050223a.xml

c1c(cc(c(c1F)F)F)F

Structure



SMIRKS Exercised

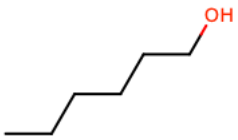
- [#1:1]-[#6X3]
- [#6:1]
- [#9:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
296.3	101.325	1	je8006474.xml

CCCCCCO

Structure



SMIRKS Exercised

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

Pure Density Data

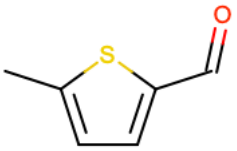
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	100	1	je501133u.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	100	1	je060248p.xml

Cc1ccc(s1)C=O

Structure



SMIRKS Exercised

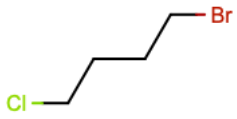
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#16:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2008.02.004.xml

C(CCBr)CCl

Structure



SMIRKS Exercised

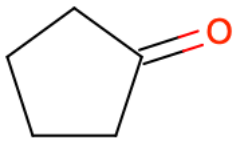
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#17:1]
- [#35:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je201002j.xml

C1CCC(=O)C1

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#6:1]
- [#6X4:1]
- [#8:1]

Pure Density Data

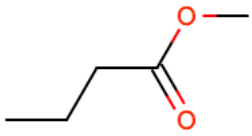
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je200468r.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je200682t.xml

CCCC(=O)OC + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

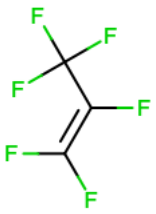
- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101.3	0.997803	0.002197	je300280s.xml

C(=C(F)F)(C(F)(F)F)F

Structure



SMIRKS Exercised

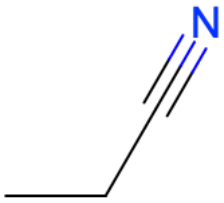
- [#6:1]
- [#6X4:1]
- [#9:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.28	100.4	1	je900596d.xml

CCC#N

Structure



SMIRKS Exercised

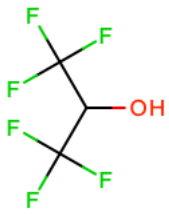
- [#1:1]-[#6X4]
- [#6X2:1]
- [#6X4:1]
- [#7:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.tca.2009.10.001.xml

C(C(F)(F)F)(C(F)(F)F)O + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

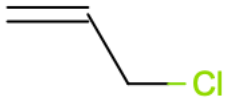
- [#1:1]-[#8]
- [#8:1]

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.205	0.795	j.jct.2011.11.019.xml
298.15	101	0.8065	0.1935	j.jct.2011.11.019.xml

C=CCCl

Structure



SMIRKS Exercised

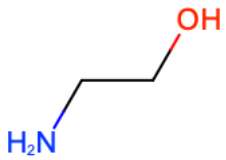
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#6:1]
- [#6X4:1]
- [#17:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
293	101.325	1	je034018b.xml

C(CO)N

Structure



SMIRKS Exercised

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

Pure Density Data

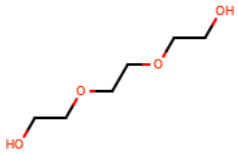
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101	1	je3013205.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101	1	j.fluid.2008.01.024.xml

C(COCCOCCO)O

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H0+0:1]
- [#8X2H1+0:1]

Pure Density Data

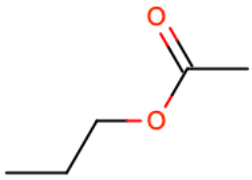
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	j.jct.2007.09.004.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	j.jct.2007.09.004.xml

CCCOC(=O)C + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

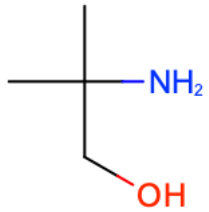
- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
318.15	101.3	0.997504	0.002496	je300280s.xml

CC(C)(CO)N

Structure



SMIRKS Exercised

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

Pure Density Data

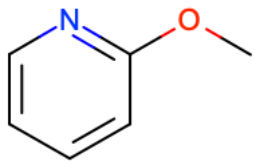
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	je050463q.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	je600515j.xml

COc1ccccn1

Structure



SMIRKS Exercised

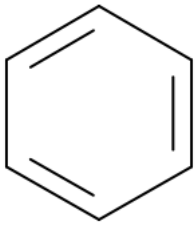
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8X2H0+0:1]
- [#7:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2011.11.032.xml

c1ccccc1

Structure



SMIRKS Exercised

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

Pure Density Data

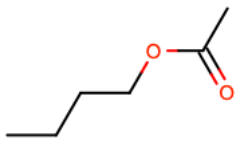
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.fluid.2008.09.005.xml

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298	101.325	1	je800091s.xml

CCCCOC(=O)C

Structure



SMIRKS Exercised

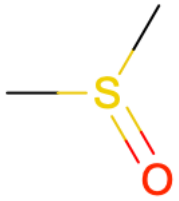
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2014.01.012.xml

CS(=O)C

Structure



SMIRKS Exercised

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

Pure Density Data

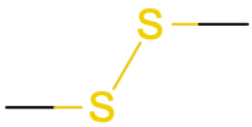
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101	1	je3007474.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101	1	je400149j.xml

CSSC

Structure



SMIRKS Exercised

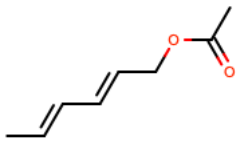
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#16:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	acs.jced.7b00078.xml

C/C=C/C=C/COC(=O)C

Structure



SMIRKS Exercised

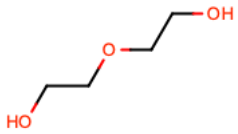
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2015.02.015.xml

C(COCCO)O

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H0+0:1]
- [#8X2H1+0:1]

Pure Density Data

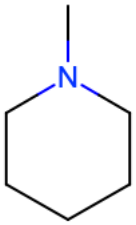
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	je300827f.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	j.jct.2007.09.004.xml

CN1CCCCC1

Structure



SMIRKS Exercised

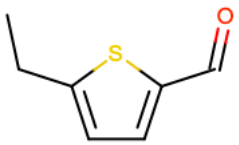
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#7:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.fluid.2010.05.001.xml

CCc1ccc(s1)C=O

Structure



SMIRKS Exercised

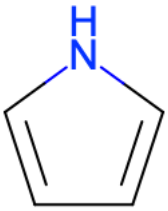
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#16:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2008.02.004.xml

c1cc[nH]c1

Structure



SMIRKS Exercised

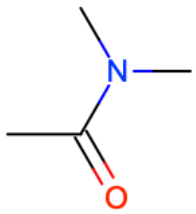
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#1:1]-[#7]
- [#6:1]
- [#7:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je700233p.xml

CC(=O)N(C)C

Structure



SMIRKS Exercised

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

Pure Density Data

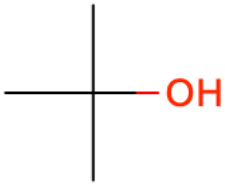
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	acs.jced.6b00354.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	j.fluid.2009.07.009.xml

CC(C)(C)O + COC=O

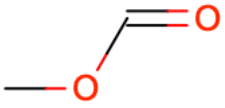
Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H1+0:1]

Structure



SMIRKS Exercised

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

Binary Enthalpy Of Mixing Data

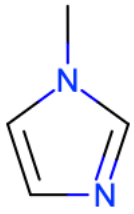
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
299.15	101.32	0.2778	0.7222	je034290l.xml
299.15	101.32	0.7127	0.2873	je034290l.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
299.15	101.32	0.2778	0.7222	je034290l.xml
299.15	101.32	0.7581	0.2419	je034290l.xml

Cn1ccnc1 + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

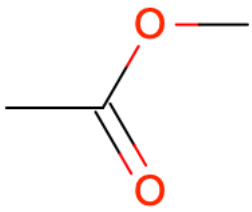
- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.006766	0.993234	je200093f.xml

CC(=O)OC

Structure



SMIRKS Exercised

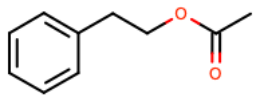
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.fluid.2015.12.029.xml

CC(=O)OCCc1ccccc1

Structure



SMIRKS Exercised

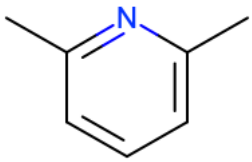
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2015.02.015.xml

Cc1cccc(n1)C

Structure



SMIRKS Exercised

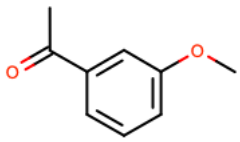
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#6:1]
- [#6X4:1]
- [#7:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je200093f.xml

CC(=O)c1cccc(c1)OC

Structure



SMIRKS Exercised

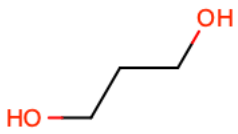
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2014.03.027.xml

C(CO)CO

Structure



SMIRKS Exercised

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

Pure Density Data

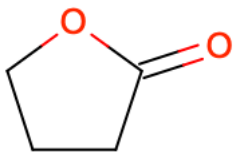
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.tca.2006.08.006.xml

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je060333x.xml

C1CC(=O)OC1

Structure



SMIRKS Exercised

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

Pure Density Data

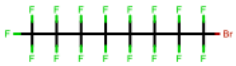
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	je100803e.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	je900503p.xml

C(C(C(C(C(F)(F)Br)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)(F)F

Structure



SMIRKS Exercised

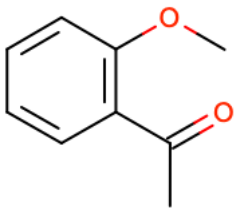
- [#6X4:1]
- [#9:1]
- [#35:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je050056e.xml

CC(=O)c1ccccc1OC

Structure



SMIRKS Exercised

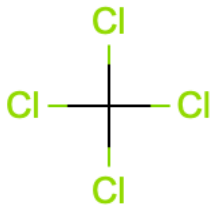
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2014.03.027.xml

C(Cl)(Cl)(Cl)Cl

Structure



SMIRKS Exercised

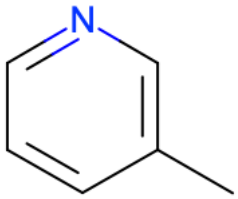
- [#6X4:1]
- [#17:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je100489z.xml

Cc1cccnc1

Structure



SMIRKS Exercised

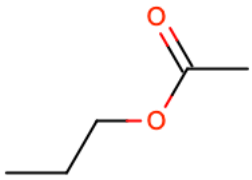
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#7:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2011.10.002.xml

CCCOC(=O)C

Structure



SMIRKS Exercised

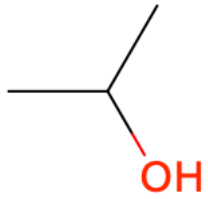
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je300974g.xml

CC(C)O

Structure



SMIRKS Exercised

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

Pure Density Data

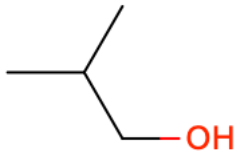
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
300.15	101.325	1	j.jct.2011.10.028.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
300.15	101.325	1	j.jct.2011.10.028.xml

CC(C)CO

Structure



SMIRKS Exercised

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

Pure Density Data

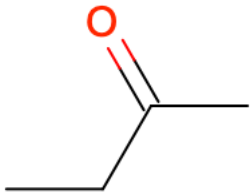
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	s10765-007-0204-0.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	je800593p.xml

CCC(=O)C + CS(=O)C

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#6:1]
- [#6X4:1]
- [#8:1]

Structure

SMIRKS Exercised

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

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2203	0.7797	j.jct.2007.04.004.xml
298.15	101	0.7615	0.2385	j.jct.2007.04.004.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
303.15	101	0.212	0.788	j.jct.2007.08.006.xml
303.15	101	0.734	0.266	j.jct.2007.08.006.xml

CCCCCCCCO

Structure

SMIRKS Exercised

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

Pure Density Data

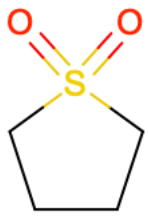
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	100	1	je400630f.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	100	1	je060248p.xml

C1CCS(=O)(=O)C1

Structure



SMIRKS Exercised

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

Pure Density Data

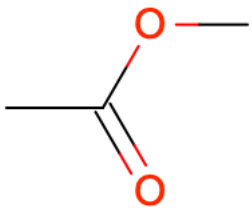
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	j.tca.2012.10.004.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	j.tca.2012.10.004.xml

CC(=O)OC + CC(C)(C)O

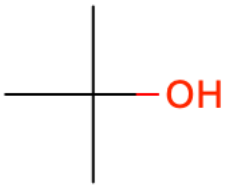
Structure



SMIRKS Exercised

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

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H1+0:1]

Binary Enthalpy Of Mixing Data

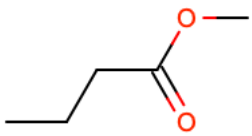
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
318.15	101.32	0.2372	0.7628	je034290l.xml
318.15	101.32	0.7696	0.2304	je034290l.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
303.15	101.32	0.2568	0.7432	je034290l.xml
303.15	101.32	0.7519	0.2481	je034290l.xml

CCCC(=O)OC

Structure



SMIRKS Exercised

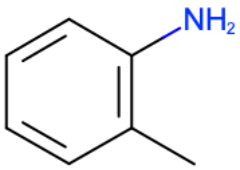
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je300280s.xml

Cc1ccccc1N + c1ccncc1

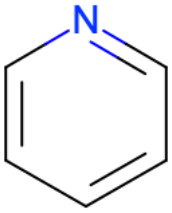
Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#7]
- [#6:1]
- [#6X4:1]
- [#7:1]

Structure



SMIRKS Exercised

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

Binary Enthalpy Of Mixing Data

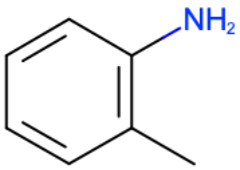
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
308.15	101	0.2681	0.7319	j.jct.2010.12.028.xml
308.15	101	0.7735	0.2265	j.jct.2010.12.028.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2374	0.7626	j.jct.2010.12.028.xml
298.15	101	0.7678	0.2322	j.jct.2010.12.028.xml

Cc1ccccc1N + Cc1ccncc1

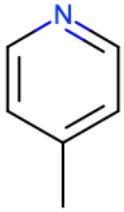
Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#7]
- [#6:1]
- [#6X4:1]
- [#7:1]

Structure



SMIRKS Exercised

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

Binary Enthalpy Of Mixing Data

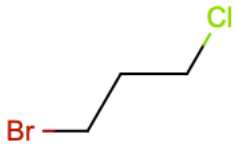
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
308.15	101	0.2715	0.7285	j.jct.2010.12.028.xml
308.15	101	0.7827	0.2173	j.jct.2010.12.028.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2655	0.7345	j.jct.2010.12.028.xml
298.15	101	0.7674	0.2326	j.jct.2010.12.028.xml

C(CCl)CBr

Structure



SMIRKS Exercised

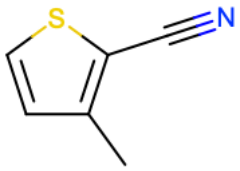
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#17:1]
- [#35:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je201002j.xml

Cc1ccsc1C#N

Structure



SMIRKS Exercised

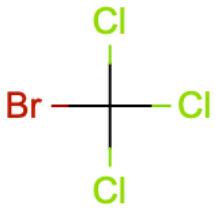
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X2:1]
- [#6X4:1]
- [#7:1]
- [#16:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2007.06.020.xml

C(Cl)(Cl)(Cl)Br

Structure



SMIRKS Exercised

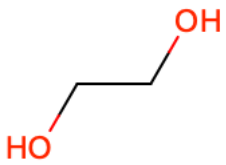
- [#6X4:1]
- [#17:1]
- [#35:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.fluid.2015.03.023.xml

C(CO)O

Structure



SMIRKS Exercised

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

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2012.08.024.xml
303.15	101.325	1	j.jct.2012.08.024.xml

Pure Enthalpy Of Vaporization Data

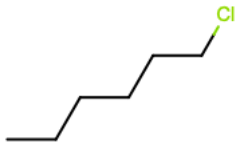
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je060333x.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	j.fluid.2009.07.009.xml

CCCCCCCl

Structure



SMIRKS Exercised

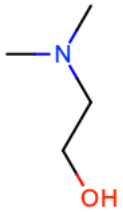
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#17:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2013.12.024.xml

CN(C)CCO

Structure



SMIRKS Exercised

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

Pure Density Data

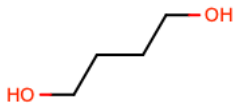
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	acs.jced.5b00282.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	j.fluid.2009.07.009.xml

C(CCO)CO

Structure



SMIRKS Exercised

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

Pure Density Data

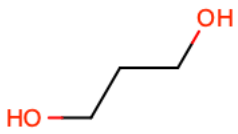
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je401020e.xml

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je060333x.xml

C(CO)CO + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

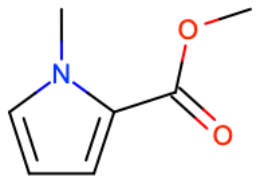
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2087	0.7913	j.jct.2005.06.018.xml
298.15	101	0.743	0.257	j.jct.2005.06.018.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2554	0.7446	j.jct.2009.11.018.xml
298.15	101	0.7551	0.2449	j.jct.2009.11.018.xml

Cn1cccc1C(=O)OC

Structure



SMIRKS Exercised

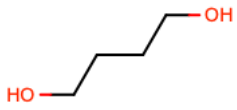
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]
- [#7:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2013.08.004.xml

C(CCO)CO + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

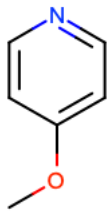
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2658	0.7342	j.jct.2005.06.018.xml
298.15	101	0.7947	0.2053	j.jct.2005.06.018.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2297	0.7703	j.jct.2009.11.018.xml
298.15	101	0.7847	0.2153	j.jct.2009.11.018.xml

COc1ccncc1

Structure



SMIRKS Exercised

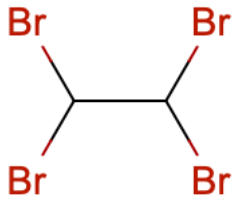
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8X2H0+0:1]
- [#7:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2011.11.032.xml

C(C(Br)Br)(Br)Br

Structure



SMIRKS Exercised

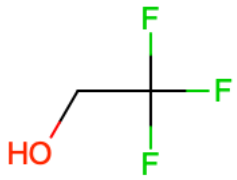
- [#1:1]-[#6X4](-[#7,#8,#9,#16,#17,#35])-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#35:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
293.15	101	1	j.jct.2005.03.027.xml

C(C(F)(F)F)O

Structure



SMIRKS Exercised

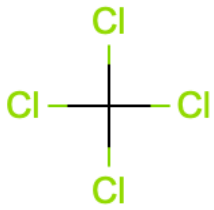
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H1+0:1]
- [#9:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je025655p.xml

C(Cl)(Cl)(Cl)Cl + CCC#N

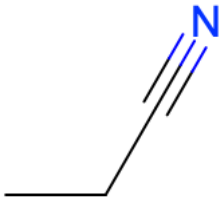
Structure



SMIRKS Exercised

- [#6X4:1]
- [#17:1]

Structure



SMIRKS Exercised

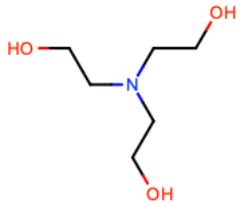
- [#1:1]-[#6X4]
- [#6X2:1]
- [#6X4:1]
- [#7:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2551	0.7449	je100489z.xml
298.15	101	0.7326	0.2674	je100489z.xml

C(CO)N(CCO)CCO

Structure



SMIRKS Exercised

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

Pure Density Data

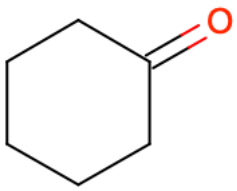
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	je050463q.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.325	1	je600515j.xml

C1CCC(=O)CC1 + CS(=O)C

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#6:1]
- [#6X4:1]
- [#8:1]

Structure

SMIRKS Exercised

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

Binary Enthalpy Of Mixing Data

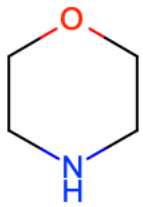
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2762	0.7238	j.jct.2007.04.004.xml
298.15	101	0.7569	0.2431	j.jct.2007.04.004.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
303.15	101	0.2241	0.7759	j.jct.2007.08.006.xml
303.15	101	0.7218	0.2782	j.jct.2007.08.006.xml

C1COCCN1

Structure



SMIRKS Exercised

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

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je020191g.xml

CO

Structure

SMIRKS Exercised

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

Pure Density Data

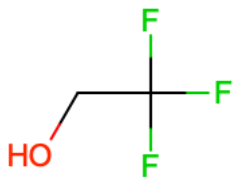
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	j.jct.2011.08.028.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101	1	je800593p.xml

C(C(F)(F)F)O + CCO

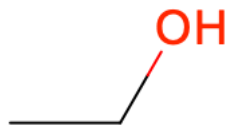
Structure



SMIRKS Exercised

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

Structure



SMIRKS Exercised

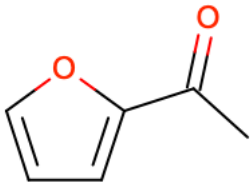
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H1+0:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.29919	0.70081	j.tca.2007.04.012.xml
298.15	101	0.79638	0.20362	j.tca.2007.04.012.xml

CC(=O)c1ccco1

Structure



SMIRKS Exercised

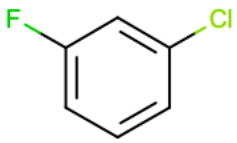
- [#1:1]-[#6X4]
- [#1:1]-[#6X3]
- [#1:1]-[#6X3] [#7,#8,#9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.jct.2008.08.004.xml

c1cc(cc(c1)Cl)F

Structure



SMIRKS Exercised

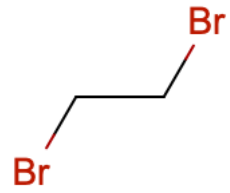
- [#1:1]-[#6X3]
- [#6:1]
- [#9:1]
- [#17:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.fluid.2014.12.023.xml

C(CBr)Br + CCCCOC=O

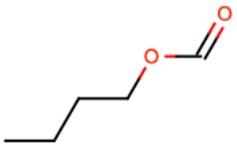
Structure



SMIRKS Exercised

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

Structure



SMIRKS Exercised

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

Binary Enthalpy Of Mixing Data

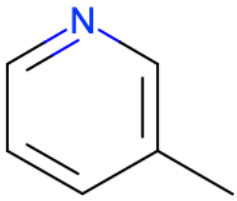
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.3993	0.6007	j.jct.2009.05.006.xml
298.15	101	0.7275	0.2725	j.jct.2009.05.006.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.3993	0.6007	j.jct.2009.05.006.xml
298.15	101	0.7738	0.2262	j.jct.2009.05.006.xml

Cc1cccnc1 + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

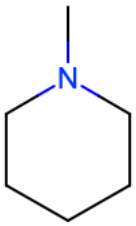
- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.005509	0.994491	je200093f.xml

CN1CCCCC1 + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

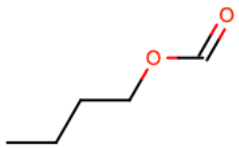
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.004409	0.995591	je200093f.xml

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.2452	0.7548	j.fluid.2010.05.001.xml
308.15	101	0.78	0.22	j.fluid.2010.05.001.xml

CCCCOC=O

Structure



SMIRKS Exercised

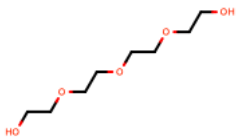
- [#1:1]-[#6X4]
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]([#7,#8,#9,#16,#17,#35]) [#7,#8, #9,#16,#17,#35]
- [#6:1]
- [#6X4:1]
- [#8:1]
- [#8X2H0+0:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	j.fluid.2013.11.026.xml

C(COCCOCCOCCO)O

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H0+0:1]
- [#8X2H1+0:1]

Pure Density Data

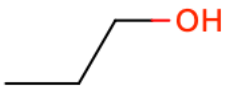
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.3	1	j.fluid.2007.09.009.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
303.15	101.3	1	j.jct.2007.09.004.xml

CCCO

Structure



SMIRKS Exercised

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

Pure Density Data

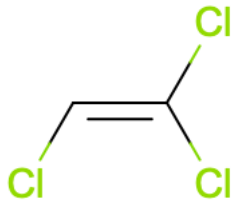
Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
300.15	101.325	1	j.jct.2011.10.028.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
300.15	101.325	1	j.jct.2011.10.028.xml

C(=C(Cl)Cl)Cl + C(CBr)Br

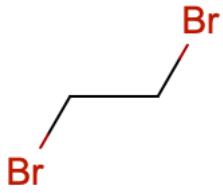
Structure



SMIRKS Exercised

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

Structure



SMIRKS Exercised

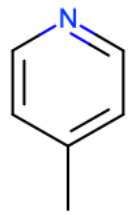
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#6X4:1]
- [#35:1]

Binary Excess Molar Volume Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
303.15	101.325	0.2077	0.7923	j.jct.2004.11.013.xml
303.15	101.325	0.7903	0.2097	j.jct.2004.11.013.xml

Cc1ccncc1 + O

Structure



SMIRKS Exercised

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

Structure

SMIRKS Exercised

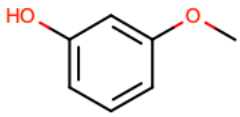
- [#1:1]-[#8]
- [#8:1]

Binary Enthalpy Of Mixing Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Mole Fraction 2	Source
298.15	101	0.005492	0.994508	je200093f.xml

COc1cccc(c1)O

Structure



SMIRKS Exercised

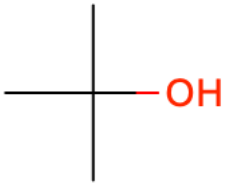
- [#1:1]-[#6X4]-[#7,#8,#9,#16,#17,#35]
- [#1:1]-[#6X3]
- [#1:1]-[#8]
- [#6:1]
- [#6X4:1]
- [#8X2H0+0:1]
- [#8X2H1+0:1]

Pure Enthalpy Of Vaporization Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	101.325	1	je025641j.xml

CC(C)(C)O

Structure



SMIRKS Exercised

- [#1:1]-[#6X4]
- [#1:1]-[#8]
- [#6X4:1]
- [#8X2H1+0:1]

Pure Density Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	100	1	j.tca.2016.03.026.xml

Pure Dielectric Constant Data

Temperature (K)	Pressure (kPa)	Mole Fraction 1	Source
298.15	100	1	je3007666.xml