In [188]:
```
%config InlineBackend.close_figures=False
%matplotlib inline
from matplotlib import interactive
interactive(False)
from sur.models import *
from sur.plots import multiplot
```

In [189]:
```
P= Mixture()
```

In [190]:
```
c= """n-pentane
n-heptane
n-nonane
n-decane
n-undecane
n-tridecane
n-pentadecane
n-hexadecane
n-octadecane
n-nonadecane
n-tricosane
n-tetracosane
n-nonacosane"""
```

In [191]:
```
f= """0,1192
0,1047
0,1124
0,0301
0,0454
0,1172
0,0948
0,0131
0,042
0,0365
0,0449
0,0066
0,2331"""
```

In [192]:
```
P.add_many(c, f)
P.sort(True)
P
```

Out[192]:
```
[(<Compound: n-PENTANE>, Decimal('0.1192')), (<Compound: n-HEPTANE>, Decimal('0.1047')),
 (<Compound: n-NONANE>, Decimal('0.1124')), (<Compound: n-DECANE>, Decimal('0.0301')), (
<Compound: n-UNDECANE>, Decimal('0.0454')), (<Compound: n-TRIDECANE>, Decimal('0.1172'))
, (<Compound: n-PENTADECANE>, Decimal('0.0948')), (<Compound: n-HEXADECANE>, Decimal('0.
0131')), (<Compound: n-OCTADECANE>, Decimal('0.042')), (<Compound: n-NONADECANE>, Decima
l('0.0365')), (<Compound: n-TRICOSANE>, Decimal('0.0449')), (<Compound: n-TETRACOSANE>,
Decimal('0.0066')), (<Compound: n-NONACOSANE>, Decimal('0.2331'))]
```

In [193]:
```
setup_P1 = EosSetup.objects.create(eos='PR', kij_mode=EosSetup.CONSTANTS,  lij_mode=EosS
etup.ZERO)

envP_PR = P.get_envelope(setup_P1, label=u"EOS PR")
```

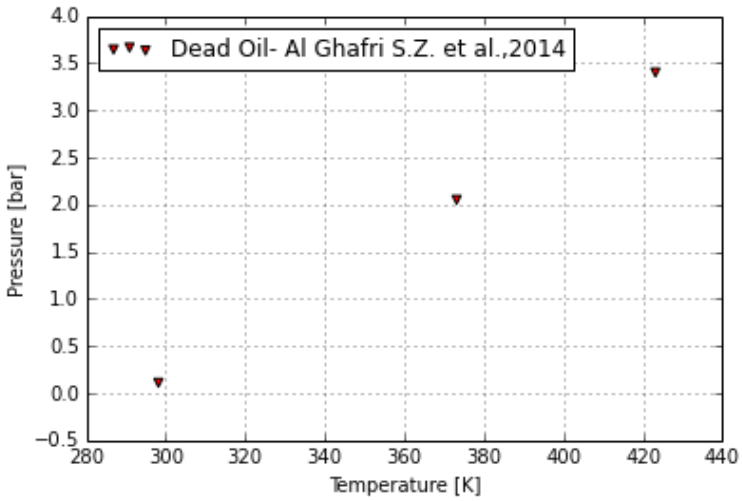
In [194]:
```
pP= """0.11 2.05 3.4"""
```

In [195]:
```
tP= """298.15 373.15 423.15"""
```

In [196]:
```
exp_envP = P.experimental_envelope(tP, pP, label=u"Dead Oil- Al Ghafri S.Z. et al.,2014"
)
```

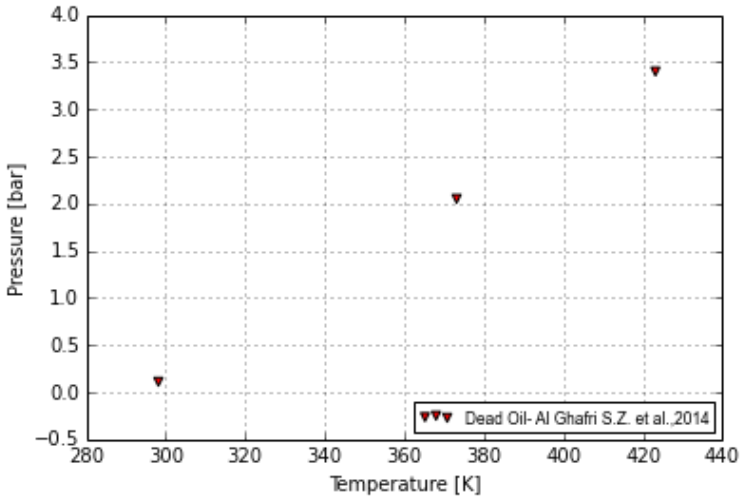
In [197]:
```
petroleo_exp= multiplot(None, [exp_envP],experimental_colors=['red'], experimental_marke
rs=['v'], legends='upper left')
petroleo_exp
```

Out[197]:



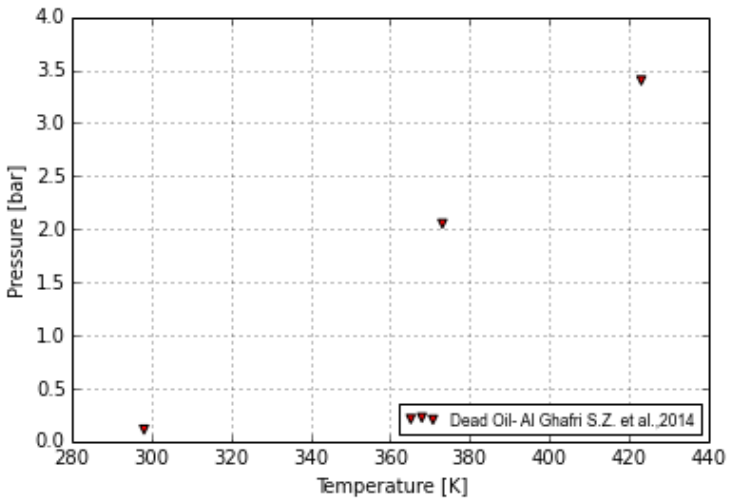
In [198]:
```
ax = petroleo_exp.get_axes()[0]

from matplotlib.font_manager import FontProperties

fontP = FontProperties()
fontP.set_size('small')
fontP.set_family('arial')
fontP.set_weight('normal')

ax.legend(loc='lower right', prop=fontP)
petroleo_exp
```

Out[198]:



In [199]:
```
ax = petroleo_exp.gca()
ax.set_ylim([0,4]),ax.grid(True)
ax.set_xlim([280,440])
petroleo_exp
```

Out[199]:



In [200]:
```
petroleo_exp.savefig('Datos experimentales de Petroleo Al-Ghafri.jpg',dpi=600)
```

In [201]:
```
for compound in P.compounds:
    print compound.delta1
    print compound._get_eos_params('RKPR')
```

```
1.95731509
[ 20.22369723   0.09363098   1.95731509   2.28798762]
2.13248282
[ 33.19200942   0.13055198   2.13248282   2.62066941]
2.22046251
[ 48.32927702   0.17068719   2.22046251   2.94387153]
2.23953806
[ 56.66107264   0.19214004   2.23953806   3.11337932]
2.2454
[ 65.63068963   0.21496967   2.2454       3.24515498]
2.2258
[ 84.92013493   0.26400572   2.2258       3.54896141]
2.1759
[ 105.78597494    0.31563822    2.1759        3.79245466]
2.1429
[ 116.42629788    0.34167676    2.1429        3.90352735]
2.0664
[ 136.47984026    0.39161949    2.0664        4.22623195]
2.0246
[ 147.18749479    0.41852655    2.0246        4.36626305]
1.8479
[ 190.85109179    0.52892198    1.8479        4.94370702]
1.8037
[ 202.2074408     0.55801882    1.8037        5.08757997]
1.5954
[ 257.96549614    0.70143907    1.5954        5.69452872]
```

In [202]:

```
c5h12 = P.compounds [0]
c5h12.delta1= 1.95731509
c5h12.save()

c7h16 = P.compounds [1]
c7h16.delta1= 2.13248282
c7h16.save()

c9h20 = P.compounds [2]
c9h20.delta1= 2.22046251
c9h20.save()

c10h22 = P.compounds [3]
c10h22.delta1= 2.23953806
c10h22.save()

c11h24= P.compounds [4]
c11h24.delta1= 2.24540237
c11h24.save()

c13h28= P.compounds [5]
c13h28.delta1= 2.22583119
c13h28.save()

c15h32= P.compounds [6]
c15h32.delta1= 2.17585934
c15h32.save()

c16h34= P.compounds [7]
c16h34.delta1= 2.14291421
c16h34.save()

c18h38= P.compounds [8]
c18h38.delta1= 2.06643905
c18h38.save()

c19h40= P.compounds [9]
c19h40.delta1= 2.02460895
c19h40.save()

c23h48= P.compounds [10]
c23h48.delta1= 1.84793231
c23h48.save()

c24h50= P.compounds [11]
c24h50.delta1= 1.8036626
c24h50.save()

c29h60= P.compounds [12]
c29h60.delta1= 1.5954152
c29h60.save()
```

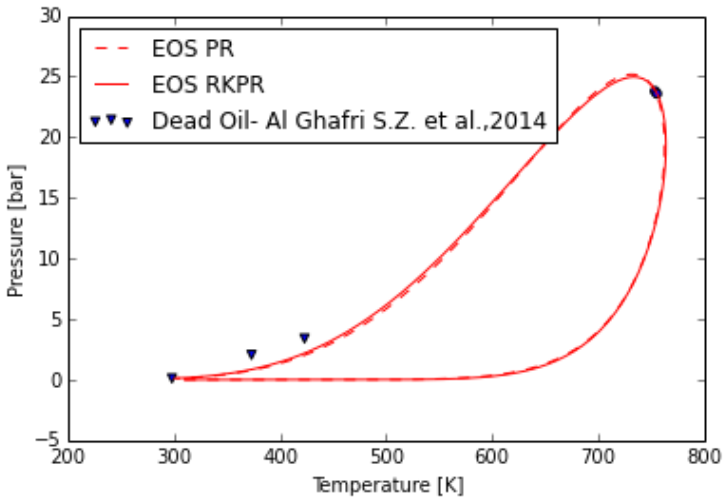
In [203]:
```
for compound in P.compounds:
    print compound.delta1
    print compound._get_eos_params('RKPR')
```

```
1.95731509
[ 20.22369723   0.09363098   1.95731509   2.28798762]
2.13248282
[ 33.19200942   0.13055198   2.13248282   2.62066941]
2.22046251
[ 48.32927702   0.17068719   2.22046251   2.94387153]
2.23953806
[ 56.66107264   0.19214004   2.23953806   3.11337932]
2.24540237
[ 65.63069744   0.21496962   2.24540237   3.24515433]
2.22583119
[ 84.92026797   0.26400504   2.22583119   3.54895264]
2.17585934
[ 105.78575868    0.31563929    2.17585934    3.79246632]
2.14291421
[ 116.4263811     0.34167636    2.14291421    3.90352325]
2.06643905
[ 136.48010839    0.39161823    2.06643905    4.22622042]
2.02460895
[ 147.18756104    0.41852624    2.02460895    4.36626039]
1.84793231
[ 190.85139985    0.52892061    1.84793231    4.94369712]
1.8036626
[ 202.20706414    0.55802048    1.8036626     5.08759148]
1.5954152
[ 257.9656867     0.70143825    1.5954152     5.6945236 ]
```

In [204]:
```
setup_P2 = EosSetup.objects.create(eos='RKPR', kij_mode=EosSetup.T_DEP,  lij_mode=EosSet
up.CONSTANTS)

for c1, c2 in combinations(P.compounds, 2):
    t = c1.tc if c1.weight < c2.weight else c2.tc
    setup_P2.set_interaction('tstar', c1, c2, t)

setup_P2.set_interaction('lij', 'n-pentane', 'n-heptane', -0.00976)
setup_P2.set_interaction('lij', 'n-pentane', 'n-nonane', -0.01498)
setup_P2.set_interaction('lij', 'n-pentane', 'n-decane', -0.01614)
setup_P2.set_interaction('lij', 'n-pentane', 'n-undecane', -0.0165)
setup_P2.set_interaction('lij', 'n-pentane', 'n-tridecane', -0.0153)
setup_P2.set_interaction('lij', 'n-pentane', 'n-pentadecane', -0.0123)
setup_P2.set_interaction('lij', 'n-pentane', 'n-hexadecane', -0.01036)
setup_P2.set_interaction('lij', 'n-pentane', 'n-octadecane', -0.00598)
setup_P2.set_interaction('lij', 'n-pentane', 'n-nonadecane', -0.00365)
setup_P2.set_interaction('lij', 'n-pentane', 'n-tricosane', 0.00568)
setup_P2.set_interaction('lij', 'n-pentane', 'n-tetracosane', 0.0079)
setup_P2.set_interaction('lij', 'n-pentane', 'n-nonacosane', 0.01773)
setup_P2.set_interaction('lij', 'n-heptane', 'n-nonane', -0.00479)
setup_P2.set_interaction('lij', 'n-heptane', 'n-decane', -0.00586)
setup_P2.set_interaction('lij', 'n-heptane', 'n-undecane', -0.00619)
setup_P2.set_interaction('lij', 'n-heptane', 'n-tridecane', -0.00509)
setup_P2.set_interaction('lij', 'n-heptane', 'n-pentadecane', -0.00234)
setup_P2.set_interaction('lij', 'n-heptane', 'n-hexadecane', -0.00055)
setup_P2.set_interaction('lij', 'n-heptane', 'n-octadecane', 0.00347)
setup_P2.set_interaction('lij', 'n-heptane', 'n-nonadecane', 0.00561)
setup_P2.set_interaction('lij', 'n-heptane', 'n-tricosane', 0.01419)
setup_P2.set_interaction('lij', 'n-heptane', 'n-tetracosane', 0.01623)
setup_P2.set_interaction('lij', 'n-heptane', 'n-nonacosane', 0.02526)
setup_P2.set_interaction('lij', 'n-nonane', 'n-decane', -0.00102)
setup_P2.set_interaction('lij', 'n-nonane', 'n-undecane', -0.00133)
setup_P2.set_interaction('lij', 'n-nonane', 'n-tridecane', -0.00028)
setup_P2.set_interaction('lij', 'n-nonane', 'n-pentadecane', 0.00235)
setup_P2.set_interaction('lij', 'n-nonane', 'n-hexadecane', 0.00406)
setup_P2.set_interaction('lij', 'n-nonane', 'n-octadecane', 0.00792)
setup_P2.set_interaction('lij', 'n-nonane', 'n-nonadecane', 0.00998)
setup_P2.set_interaction('lij', 'n-nonane', 'n-tricosane', 0.0182)
setup_P2.set_interaction('lij', 'n-nonane', 'n-tetracosane', 0.02016)
setup_P2.set_interaction('lij', 'n-nonane', 'n-nonacosane', 0.02881)
setup_P2.set_interaction('lij', 'n-decane', 'n-undecane', -0.00031)
setup_P2.set_interaction('lij', 'n-decane', 'n-tridecane', 0.00072)
setup_P2.set_interaction('lij', 'n-decane', 'n-pentadecane', 0.00334)
setup_P2.set_interaction('lij', 'n-decane', 'n-hexadecane', 0.00504)
setup_P2.set_interaction('lij', 'n-decane', 'n-octadecane', 0.00886)
setup_P2.set_interaction('lij', 'n-decane', 'n-nonadecane', 0.0109)
setup_P2.set_interaction('lij', 'n-decane', 'n-tricosane', 0.01905)
setup_P2.set_interaction('lij', 'n-decane', 'n-tetracosane', 0.02099)
setup_P2.set_interaction('lij', 'n-decane', 'n-nonacosane', 0.02956)
setup_P2.set_interaction('lij', 'n-undecane', 'n-tridecane', 0.00104)
setup_P2.set_interaction('lij', 'n-undecane', 'n-pentadecane', 0.00365)
setup_P2.set_interaction('lij', 'n-undecane', 'n-hexadecane', 0.00534)
setup_P2.set_interaction('lij', 'n-undecane', 'n-octadecane', 0.00915)
```

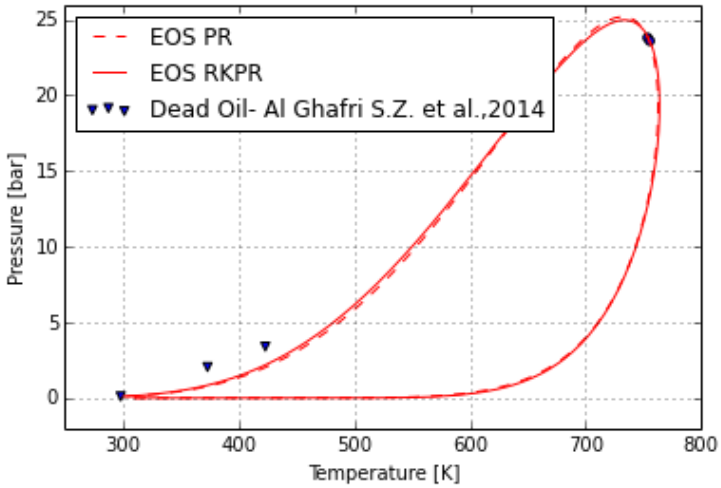
In [205]:
```
Caso_Petroleo= multiplot([envP_PR, envP_RKPR],[exp_envP], formats=['--r','r'], experimen
tal_colors=['b'],experimental_markers=['v'],legends='best')
Caso_Petroleo
```

Out[205]:



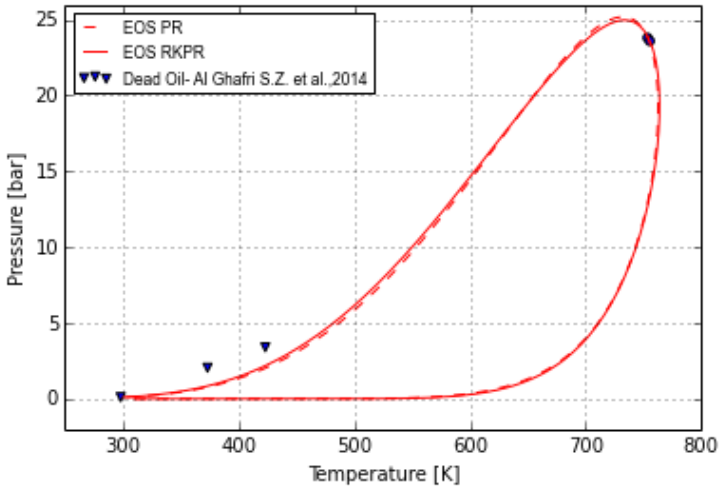
In [206]:
```
ax = Caso_Petroleo.gca()
ax.set_ylim([-2,26]),ax.grid(True)
ax.set_xlim([250,800])
Caso_Petroleo
```

Out[206]:



In [207]:
```
ax = Caso_Petroleo.get_axes()[0]
Caso_Petroleo

from matplotlib.font_manager import FontProperties

fontP = FontProperties()
fontP.set_size('small')
fontP.set_family('arial')
fontP.set_weight('normal')

ax.legend(loc='upper left', prop=fontP)
Caso_Petroleo
```

Out[207]:



In [208]:
```
Caso_Petroleo.savefig('Dead oil-Al Ghafri_2014.jpg', dpi=600)
```

In [209]:
```
LiveOil= Mixture()
```

In [210]:
```
elementos= ['n-pentane','n-heptane','n-nonane','n-decane','n-undecane','n-tridecane','n-
pentadecane','n-hexadecane','n-octadecane','n-nonadecane','n-tricosane','n-tetracosane',
'n-nonacosane','methane','ethane','propane']
fracciones= [0.0714,0.0628,0.0675,0.0181,0.0272,0.0703,0.0569,0.0079,0.0252,0.0219,0.026
9,0.004,0.1399,0.3252,0.0504,0.0244]

for elemento, fraccion in zip(elementos, fracciones):
    LiveOil[elemento]= fraccion
```

In [211]:
```
LiveOil.sort(True)
LiveOil
```

Out[211]:
```
[(<Compound: METHANE>, Decimal('0.3252')), (<Compound: ETHANE>, Decimal('0.0504')), (<Co
mpound: PROPANE>, Decimal('0.0244')), (<Compound: n-PENTANE>, Decimal('0.0714')), (<Comp
ound: n-HEPTANE>, Decimal('0.0628')), (<Compound: n-NONANE>, Decimal('0.0675')), (<Compo
und: n-DECANE>, Decimal('0.0181')), (<Compound: n-UNDECANE>, Decimal('0.0272')), (<Compo
und: n-TRIDECANE>, Decimal('0.0703')), (<Compound: n-PENTADECANE>, Decimal('0.0569')), (
<Compound: n-HEXADECANE>, Decimal('0.0079')), (<Compound: n-OCTADECANE>, Decimal('0.0252
')), (<Compound: n-NONADECANE>, Decimal('0.0219')), (<Compound: n-TRICOSANE>, Decimal('0
.0269')), (<Compound: n-TETRACOSANE>, Decimal('0.004')), (<Compound: n-NONACOSANE>, Deci
mal('0.1399'))]
```

In [212]:
```
for compound in LiveOil.compounds:
    print compound.delta1
    print compound._get_eos_params('RKPR')
```

```
0.5
[ 2.30376808  0.0304338   0.5         1.54083759]
0.8
[ 5.61628283  0.04561112  0.8         1.90385075]
1.6
[ 9.77170891  0.06017136  1.6         1.96439211]
1.95731509
[ 20.22369723   0.09363098   1.95731509   2.28798762]
2.13248282
[ 33.19200942   0.13055198   2.13248282   2.62066941]
2.22046251
[ 48.32927702   0.17068719   2.22046251   2.94387153]
2.23953806
[ 56.66107264   0.19214004   2.23953806   3.11337932]
2.24540237
[ 65.63069744   0.21496962   2.24540237   3.24515433]
2.22583119
[ 84.92026797   0.26400504   2.22583119   3.54895264]
2.17585934
[ 105.78575868    0.31563929    2.17585934    3.79246632]
2.14291421
[ 116.4263811     0.34167636    2.14291421    3.90352325]
2.06643905
[ 136.48010839    0.39161823    2.06643905    4.22622042]
2.02460895
[ 147.18756104    0.41852624    2.02460895    4.36626039]
1.84793231
[ 190.85139985    0.52892061    1.84793231    4.94369712]
1.8036626
[ 202.20706414    0.55802048    1.8036626     5.08759148]
1.5954152
[ 257.9656867     0.70143825    1.5954152     5.6945236 ]
```

In [213]:
```
methane = LiveOil.compounds [0]
methane.delta1 = 0.50
methane.save()

c2h6= LiveOil.compounds[1]
c2h6.delta1= 0.8
c2h6.save()

c3h8= LiveOil.compounds[2]
c3h8.delta1= 1.6
c3h8.save()

c5h12= LiveOil.compounds[3]
c5h12.delta1= 1.9573
c5h12.save()

c7h16= LiveOil.compounds[4]
c7h16.delta1= 2.1325
c7h16.save()

c9h20= LiveOil.compounds[5]
c9h20.delta1= 2.2205
c9h20.save()

c10h22= LiveOil.compounds[6]
c10h22.delta1= 2.2395
c10h22.save()

c11h24= LiveOil.compounds[7]
c11h24.delta1= 2.2454
c11h24.save()

c13h28= LiveOil.compounds[8]
c13h28.delta1= 2.2258
c13h28.save()

c15h32= LiveOil.compounds[9]
c15h32.delta1= 2.1759
c15h32.save()

c16h34= LiveOil.compounds[10]
c16h34.delta1= 2.1429
c16h34.save()

c18h38= LiveOil.compounds[11]
c18h38.delta1= 2.0664
c18h38.save()

c19h40= LiveOil.compounds[12]
c19h40.delta1= 2.0246
c19h40.save()

c23h48= LiveOil.compounds[13]
```

In [214]:
```
for compound in LiveOil.compounds:
    print compound.delta1
    print compound._get_eos_params('RKPR')
```

```
0.5
[ 2.30376808  0.0304338   0.5         1.54083759]
0.8
[ 5.61628283  0.04561112  0.8         1.90385075]
1.6
[ 9.77170891  0.06017136  1.6         1.96439211]
1.9573
[ 20.2236819    0.0936311    1.9573       2.28799136]
2.1325
[ 33.19203811   0.13055179   2.1325       2.62066497]
2.2205
[ 48.32936804   0.17068666   2.2205       2.94386153]
2.2395
[ 56.66096436   0.19214065   2.2395       3.11338964]
2.2454
[ 65.63068963   0.21496967   2.2454       3.24515498]
2.2258
[ 84.92013493   0.26400572   2.2258       3.54896141]
2.1759
[ 105.78597494    0.31563822    2.1759        3.79245466]
2.1429
[ 116.42629788    0.34167676    2.1429        3.90352735]
2.0664
[ 136.47984026    0.39161949    2.0664        4.22623195]
2.0246
[ 147.18749479    0.41852655    2.0246        4.36626305]
1.8479
[ 190.85109179    0.52892198    1.8479        4.94370702]
1.8037
[ 202.2074408     0.55801882    1.8037        5.08757997]
1.5954
[ 257.96549614    0.70143907    1.5954        5.69452872]
```

In [215]:
```
setup_RKPR_LiveOil = EosSetup.objects.create(eos='RKPR', kij_mode=EosSetup.T_DEP,  lij_m
ode=EosSetup.CONSTANTS)

for c1, c2 in combinations(LiveOil.compounds, 2):
    t = c1.tc if c1.weight < c2.weight else c2.tc
    setup_RKPR_LiveOil.set_interaction('tstar', c1, c2, t)

setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'ethane', 0.00307)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'propane', 0.01)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-pentane', 0.03022)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-heptane', 0.04678)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-nonane', 0.06183)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-decane', 0.06853)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-undecane', 0.07471)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-tridecane', 0.08508)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-pentadecane', 0.09292)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-hexadecane', 0.09592)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-octadecane', 0.10024)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-nonadecane', 0.10199)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-tricosane', 0.10647)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-tetracosane', 0.10717)
setup_RKPR_LiveOil.set_interaction('k0', 'methane', 'n-nonacosane', 0.10912)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'ethane', -0.0079)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'propane', -0.04225)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-pentane', -0.08473)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-heptane', -0.11875)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-nonane', -0.14036)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-decane', -0.14551)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-undecane', -0.14713)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-tridecane', -0.14179)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-pentadecane', -0.12897)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-hexadecane', -0.12114)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-octadecane', -0.10465)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-nonadecane', -0.09655)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-tricosane', -0.06835)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-tetracosane', -0.06259)
setup_RKPR_LiveOil.set_interaction('lij', 'methane', 'n-nonacosane', -0.0409)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'propane', -0.00437)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-pentane', -0.00616)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-heptane', -0.00967)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-nonane', -0.0121)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-decane', -0.01269)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-undecane', -0.01288)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-tridecane', -0.01226)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-pentadecane', -0.0108)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-hexadecane', -0.00993)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-octadecane', -0.00817)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-nonadecane', -0.00733)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-tricosane', -0.00462)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-tetracosane', -0.0041)
setup_RKPR_LiveOil.set_interaction('lij', 'ethane', 'n-nonacosane', -0.00231)
setup_RKPR_LiveOil.set_interaction('lij', 'propane', 'n-pentane', -0.02082)
setup_RKPR_LiveOil.set_interaction('lij', 'propane', 'n-heptane', -0.03242)
```

In [216]:
```
setup_PR_LiveOil = EosSetup.objects.create(eos='PR', kij_mode=EosSetup.CONSTANTS,  lij_m
ode=EosSetup.ZERO)

setup_PR_LiveOil.set_interaction('kij', 'methane', 'ethane', 0.01141)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'propane', 0.01671)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-pentane', 0.02654)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-heptane', 0.03543)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-nonane', 0.04348)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-decane', 0.04721)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-undecane', 0.05076)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-tridecane', 0.05735)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-pentadecane', 0.06331)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-hexadecane', 0.06608)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-octadecane', 0.07121)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-nonadecane', 0.07359)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-tricosane', 0.082)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-tetracosane', 0.08385)
setup_PR_LiveOil.set_interaction('kij', 'methane', 'n-nonacosane', 0.09185)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'propane', 0.0011)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'n-pentane', 0.0078)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'n-heptane', 0.015)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'n-nonane', 0.019)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'n-decane', 0.03)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'n-undecane', 0.03)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'n-tridecane', 0.03)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'n-pentadecane', 0.04)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'n-hexadecane', 0.04)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'n-octadecane', 0.04)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'n-nonadecane', 0.04)
setup_PR_LiveOil.set_interaction('kij', 'ethane', 'n-tricosane', 0.05)
setup_PR_LiveOil.set_interaction('kij', 'propane', 'n-pentane', 0.012)
setup_PR_LiveOil.set_interaction('kij', 'propane', 'n-heptane', 0.056)
setup_PR_LiveOil.set_interaction('kij', 'propane', 'n-nonane', 0.007)
setup_PR_LiveOil.set_interaction('kij', 'propane', 'n-decane', 0.02)
setup_PR_LiveOil.set_interaction('kij', 'propane', 'n-undecane', 0.02)
setup_PR_LiveOil.set_interaction('kij', 'propane', 'n-tridecane', 0.02)
setup_PR_LiveOil.set_interaction('kij', 'propane', 'n-pentadecane', 0.025)
setup_PR_LiveOil.set_interaction('kij', 'propane', 'n-hexadecane', 0.025)
setup_PR_LiveOil.set_interaction('kij', 'propane', 'n-octadecane', 0.025)
setup_PR_LiveOil.set_interaction('kij', 'propane', 'n-nonadecane', 0.025)
setup_PR_LiveOil.set_interaction('kij', 'propane', 'n-tricosane', 0.03)

envLiveOil_PR = LiveOil.get_envelope(setup_PR_LiveOil, label=u"EOS PR")
```

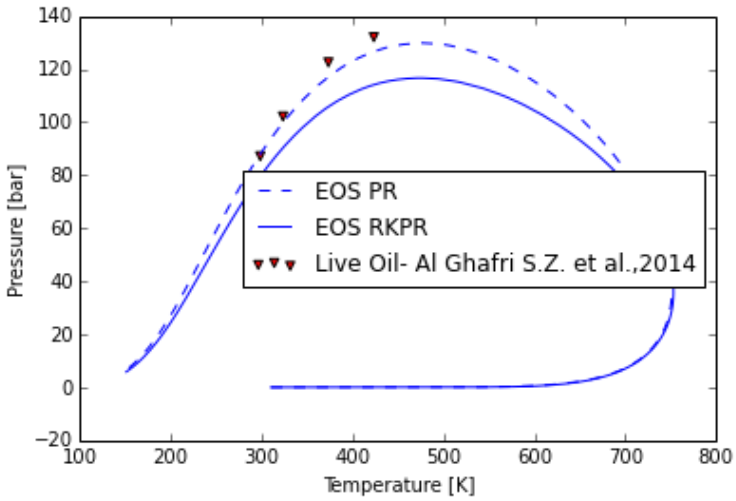
In [217]:
```
TLO= """298.15 323.15 373.15 423.15"""
```

In [218]:
```
PLO= """87.10 102.10 122.50 132"""
```

In [219]:
```
exp_envLiveOil = LiveOil.experimental_envelope(TLO, PLO, label=u"Live Oil- Al Ghafri S.Z
. et al.,2014")
```

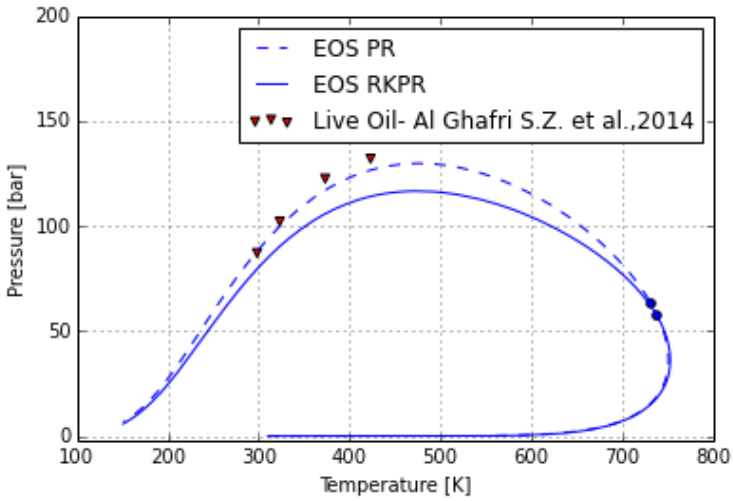
In [220]:
```
Caso_LiveOil= multiplot([envLiveOil_PR, envLiveOil_RKPR],[exp_envLiveOil], formats=['--b
','b'],experimental_colors=['r'], experimental_markers=['v'], legends='best')
Caso_LiveOil
```

Out[220]:



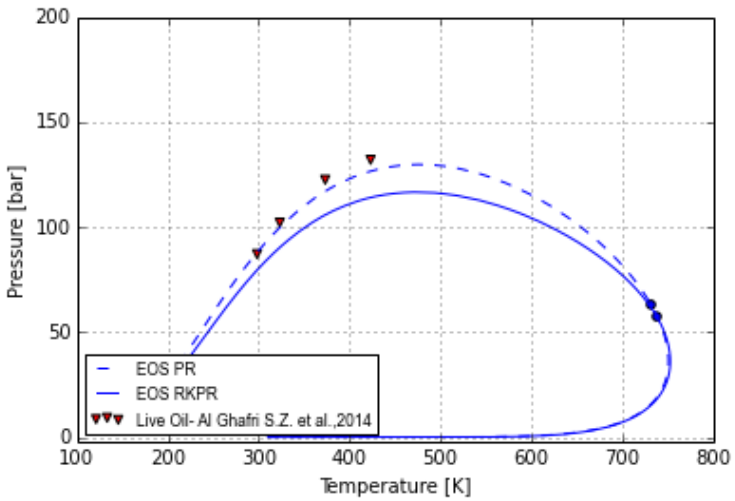
In [221]:
```
ax = Caso_LiveOil.gca()
ax.set_ylim([-2,200]),ax.grid(True)
Caso_LiveOil
```

Out[221]:



In [222]:
```
ax = Caso_LiveOil.get_axes()[0]

from matplotlib.font_manager import FontProperties

fontP = FontProperties()
fontP.set_size('small')
fontP.set_family('arial')
fontP.set_weight('normal')

ax.legend(loc='lower left', prop=fontP)
Caso_LiveOil
```

Out[222]:



In [223]:
```
A= Mixture()
```

In [224]:
```
elementos= ['methane','n-pentane','n-heptane','n-octane','n-decane','n-undecane','n-dode
cane','n-pentadecane','n-octadecane','n-nonadecane','n-hexatriacontane','n-hexadecane']
fracciones= [0.404, 0.2723,0.0163,0.1308,0.0828,0.037,0.0171,0.0083,0.0102,0.0023,0.0015
5,0.0174]

for elemento, fraccion in zip(elementos, fracciones):
    A[elemento]= fraccion
```

In [225]:
```
A.sort(True)
A
```

Out[225]:
```
[(<Compound: METHANE>, Decimal('0.404')), (<Compound: n-PENTANE>, Decimal('0.2723')), (<
Compound: n-HEPTANE>, Decimal('0.0163')), (<Compound: n-OCTANE>, Decimal('0.1308')), (<C
ompound: n-DECANE>, Decimal('0.0828')), (<Compound: n-UNDECANE>, Decimal('0.037')), (<Co
mpound: n-DODECANE>, Decimal('0.0171')), (<Compound: n-PENTADECANE>, Decimal('0.0083')),
 (<Compound: n-HEXADECANE>, Decimal('0.01735')), (<Compound: n-OCTADECANE>, Decimal('0.0
102')), (<Compound: n-NONADECANE>, Decimal('0.0023')), (<Compound: n-HEXATRIACONTANE>, D
ecimal('0.00155'))]
```

In [226]:
```
for compound in A.compounds:
    print compound.delta1
    print compound._get_eos_params('RKPR')
```

```
0.5
[ 2.30376808  0.0304338   0.5         1.54083759]
1.9573
[ 20.2236819    0.0936311    1.9573       2.28799136]
2.1325
[ 33.19203811   0.13055179   2.1325       2.62066497]
2.18571421
[ 40.58865788   0.15057346   2.18571421   2.79307492]
2.2395
[ 56.66096436   0.19214065   2.2395       3.11338964]
2.2454
[ 65.63068963   0.21496967   2.2454       3.24515498]
2.2402
[ 74.54300191   0.23727573   2.2402       3.40567106]
2.1759
[ 105.78597494    0.31563822    2.1759        3.79245466]
2.1429
[ 116.42629788    0.34167676    2.1429        3.90352735]
2.0664
[ 136.47984026    0.39161949    2.0664        4.22623195]
2.0246
[ 147.18749479    0.41852655    2.0246        4.36626305]
1.3603
[ 337.07505774    0.90434304    1.3603        6.44792963]
```

In [227]:

```
methane= A.compounds[0]
methane.delta1= 0.5
methane.save()

c5h12= A.compounds[1]
c5h12.delta1= 1.9573
c5h12.save()

c7h16= A.compounds[2]
c7h16.delta1= 2.1325
c7h16.save()

c8h18= A.compounds[3]
c8h18.delta1= 2.1857
c8h18.save()

c10h22= A.compounds[4]
c10h22.delta1= 2.2395
c10h22.save()

c11h24= A.compounds[5]
c11h24.delta1= 2.2454
c11h24.save()

c12h26= A.compounds[6]
c12h26.delta1= 2.2402
c12h26.save()

c15h32= A.compounds[7]
c15h32.delta1= 2.1759
c15h32.save()

c16h34= A.compounds[8]
c16h34.delta1= 2.1429
c16h34.save()

c18h38= A.compounds[9]
c18h38.delta1= 2.0664
c18h38.save()

c19h40= A.compounds[10]
c19h40.delta1= 2.0246
c19h40.save()

c36h74= A.compounds[11]
c36h74.delta1= 1.3603
c36h74.save()
```

In [228]:
```
setupA_RKPR = EosSetup.objects.create(eos='RKPR', kij_mode=EosSetup.T_DEP,  lij_mode=Eos
Setup.CONSTANTS)

for c1, c2 in combinations(A.compounds, 2):
    t = c1.tc if c1.weight < c2.weight else c2.tc
    setupA_RKPR.set_interaction('tstar', c1, c2, t)

setupA_RKPR.set_interaction('k0', 'methane', 'n-pentane', 0.03022)
setupA_RKPR.set_interaction('k0', 'methane', 'n-heptane', 0.04678)
setupA_RKPR.set_interaction('k0', 'methane', 'n-octane', 0.05464)
setupA_RKPR.set_interaction('k0', 'methane', 'n-decane', 0.06853)
setupA_RKPR.set_interaction('k0', 'methane', 'n-undecane', 0.07472)
setupA_RKPR.set_interaction('k0', 'methane', 'n-dodecane', 0.07995)
setupA_RKPR.set_interaction('k0', 'methane', 'n-pentadecane', 0.09292)
setupA_RKPR.set_interaction('k0', 'methane', 'n-hexadecane', 0.09593)
setupA_RKPR.set_interaction('k0', 'methane', 'n-octadecane', 0.10025)
setupA_RKPR.set_interaction('k0', 'methane', 'n-nonadecane', 0.10199)
setupA_RKPR.set_interaction('k0', 'methane', 'n-hexatriacontane', 0.10999)

setupA_RKPR.set_interaction('lij', 'methane', 'n-pentane', -0.08474)
setupA_RKPR.set_interaction('lij', 'methane', 'n-heptane', -0.11875)
setupA_RKPR.set_interaction('lij', 'methane', 'n-octane', -0.13141)
setupA_RKPR.set_interaction('lij', 'methane', 'n-decane', -0.14036)
setupA_RKPR.set_interaction('lij', 'methane', 'n-undecane', -0.14714)
setupA_RKPR.set_interaction('lij', 'methane', 'n-dodecane', -0.1457)
setupA_RKPR.set_interaction('lij', 'methane', 'n-pentadecane', -0.12898)
setupA_RKPR.set_interaction('lij', 'methane', 'n-hexadecane', -0.12114)
setupA_RKPR.set_interaction('lij', 'methane', 'n-octadecane', -0.10465)
setupA_RKPR.set_interaction('lij', 'methane', 'n-nonadecane', -0.09655)
setupA_RKPR.set_interaction('lij', 'methane', 'n-hexatriacontane', -0.02447)

setupA_RKPR.set_interaction('lij', 'n-pentane', 'n-heptane', -0.009761)
setupA_RKPR.set_interaction('lij', 'n-pentane', 'n-octane', -0.012895)
setupA_RKPR.set_interaction('lij', 'n-pentane', 'n-decane', -0.016146)
setupA_RKPR.set_interaction('lij', 'n-pentane', 'n-undecane', -0.016505)
setupA_RKPR.set_interaction('lij', 'n-pentane', 'n-dodecane', -0.016187)
setupA_RKPR.set_interaction('lij', 'n-pentane', 'n-pentadecane', -0.012308)
setupA_RKPR.set_interaction('lij', 'n-pentane', 'n-hexadecane', -0.010369)
setupA_RKPR.set_interaction('lij', 'n-pentane', 'n-octadecane', -0.005984)
setupA_RKPR.set_interaction('lij', 'n-pentane', 'n-nonadecane', -0.003653)
setupA_RKPR.set_interaction('lij', 'n-pentane', 'n-hexatriacontane', 0.027703)

setupA_RKPR.set_interaction('lij', 'n-heptane', 'n-octane', -0.00288)
setupA_RKPR.set_interaction('lij', 'n-heptane', 'n-decane', -0.005867)
setupA_RKPR.set_interaction('lij', 'n-heptane', 'n-undecane', -0.006198)
setupA_RKPR.set_interaction('lij', 'n-heptane', 'n-dodecane', -0.005905)
setupA_RKPR.set_interaction('lij', 'n-heptane', 'n-pentadecane', -0.002341)
setupA_RKPR.set_interaction('lij', 'n-heptane', 'n-hexadecane', -0.000558)
setupA_RKPR.set_interaction('lij', 'n-heptane', 'n-octadecane', 0.003471)
setupA_RKPR.set_interaction('lij', 'n-heptane', 'n-nonadecane', 0.005613)
setupA_RKPR.set_interaction('lij', 'n-heptane', 'n-hexatriacontane', 0.034428)

setupA_RKPR.set_interaction('lij', 'n-octane', 'n-decane', -0.002912)
```

In [229]:
```
setupA_PR = EosSetup.objects.create(eos='PR', kij_mode=EosSetup.CONSTANTS,  lij_mode=Eos
Setup.ZERO)

setupA_PR.set_interaction('Kij', 'methane', 'n-pentane', 0.0265)
setupA_PR.set_interaction('Kij', 'methane', 'n-heptane', 0.0354)
setupA_PR.set_interaction('Kij', 'methane', 'n-octane', 0.0395)
setupA_PR.set_interaction('Kij', 'methane', 'n-decane', 0.0472)
setupA_PR.set_interaction('Kij', 'methane', 'n-undecane', 0.0507)
setupA_PR.set_interaction('Kij', 'methane', 'n-dodecane', 0.0541)
setupA_PR.set_interaction('Kij', 'methane', 'n-pentadecane', 0.0633)
setupA_PR.set_interaction('Kij', 'methane', 'n-hexadecane', 0.066)
setupA_PR.set_interaction('Kij', 'methane', 'n-octadecane', 0.0712)
setupA_PR.set_interaction('Kij', 'methane', 'n-nonadecane', 0.0735)

envA_PR= A.get_envelope(setupA_PR, label=u"EOS PR")
```

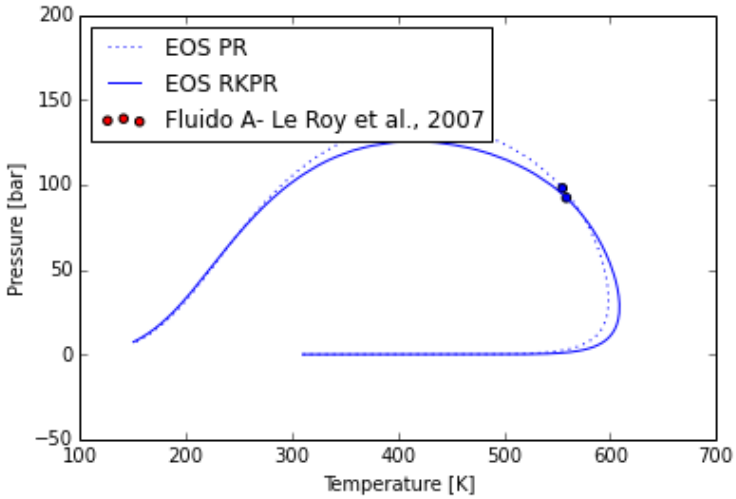
In [230]:
```
tA="""323 373 413"""
```

In [231]:
```
pA="""146 163 169"""
```

In [232]:
```
exp_envA = A.experimental_envelope(tA, pA, label=u"Fluido A- Le Roy et al., 2007")
```

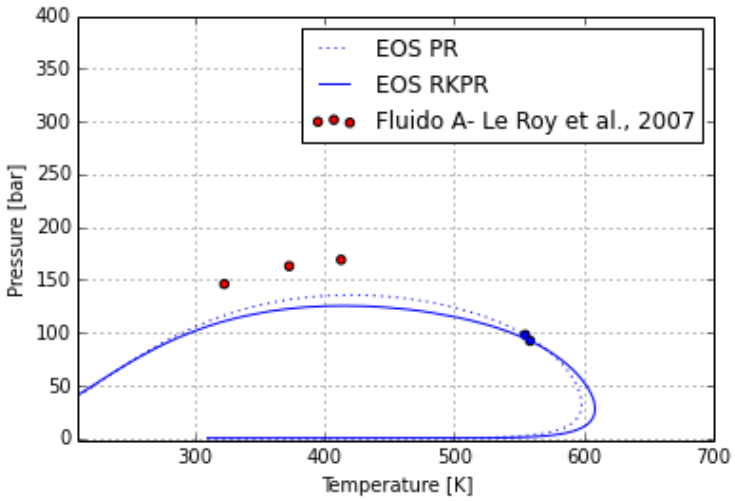
In [233]:
```
fluido_A= multiplot([envA_PR,envA_RKPR],[exp_envA],formats=[':b','b'],experimental_color
s=['red'], experimental_markers=['o'], legends='best')
fluido_A
```

Out[233]:



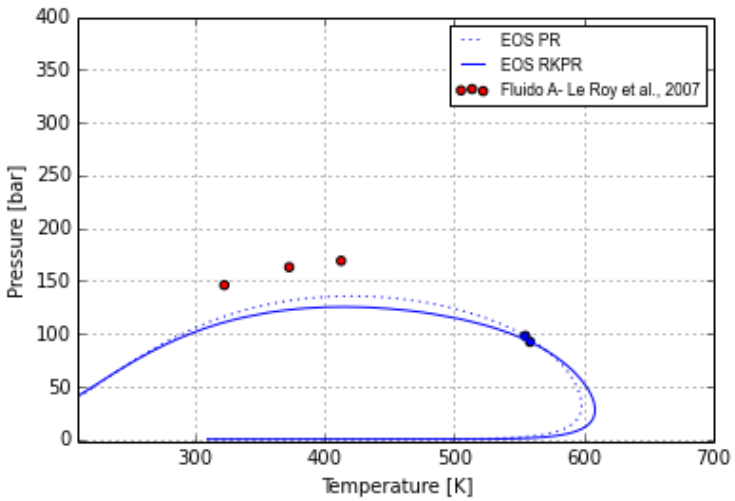
In [234]:
```
ax = fluido_A.gca()
ax.set_ylim([-2,400]),ax.grid(True)
ax.set_xlim([210,700])
fluido_A
```

Out[234]:



In [235]:
```
ax = fluido_A.get_axes()[0]
fluido_A

from matplotlib.font_manager import FontProperties

fontP = FontProperties()
fontP.set_size('small')
fontP.set_family('arial')
fontP.set_weight('normal')

ax.legend(loc='upper right', prop=fontP)
fluido_A
```

Out[235]:



In [236]:
```
fluido_A.savefig('live oil-le roy mezcla A.jpg',dpi=900)
```

In [237]:
```
Caso_LiveOil.savefig('live oil al ghafri.jpg',dpi=900)
```

In [238]:
```
GC= Mixture()
```

In [239]:
```
elementos= ['methane', 'n-butane', 'n-heptane', 'n-decane', 'n-tetradecane']
fracciones= [0.80, 0.14, 0.04, 0.014, 0.006]

for elemento, fraccion in zip(elementos, fracciones):
    GC[elemento]= fraccion
```

In [240]:
```
GC.sort(True)
GC
```

Out[240]:
```
[(<Compound: METHANE>, Decimal('0.8')), (<Compound: n-BUTANE>, Decimal('0.14')), (<Compo
und: n-HEPTANE>, Decimal('0.04')), (<Compound: n-DECANE>, Decimal('0.014')), (<Compound:
 n-TETRADECANE>, Decimal('0.006'))]
```

In [241]:
```
setup_GC1 = EosSetup.objects.create(eos='PR', kij_mode=EosSetup.CONSTANTS,  lij_mode=Eos
Setup.ZERO)
```

In [242]:
```
MatrizGC = """0 0.0218 0.0354 0.0472 0.0604
0 0 0 0 0
0 0 0 0 0
0 0 0 0 0
0 0 0 0 0"""
```

In [243]:
```
setup_GC1.set_interaction_matrix('kij', GC, MatrizGC)
```

In [244]:
```
envGC_PR = GC.get_envelope(setup_GC1, label=u"EOS PR")
```

In [245]:
```
pGC= """147.44 153.79 160.59 166.59 172.64 177.94 183.09 183.69 183.99 184.59 185.24 185
.69 187.64 191.74
195.64 199.09 202.34 205.09 207.64 209.89 211.79 213.29 215.79 216.24 215.44 213.34 210.
49 205.39 204.24
202.49 199.29 195.59 191.19 188.99 186.79 30.67 35.65 40.64 45.63 50.62 55.62 60.61 65.6
1 70.61 75.60
80.60 85.60 90.60 95.60 100.60 105.60 110.60 115.60 120.60 125.60 130.59 110.59 120.59 1
30.60 135.60
140.60 145.60 150.60 155.60 160.60 165.60 170.60 14.09 14.59 15.59 16.58 18.08 20.57 23.
06 25.54 28.04
30.53 33.04 35.53 40.53 45.53 50.53 55.53 60.53 65.53 70.53"""
```

In [246]:
```
tGC= """244.62 248.99 253.99 258.70 263.75 268.57 273.72 274.35 274.75 275.31 276.08
276.50 278.74 283.60 288.64 293.52 298.61 303.42 308.48 313.60 318.45 323.28 338.20 346.
76 357.47
368.27 378.00 388.49 390.68 393.32 398.35 403.4 408.51 411.12 413.81 456.51 459.01 460.8
1 462.36
463.78 464.69 465.26 465.33 465.21 464.84 464.54 464.26 463.69 462.33 461.00 459.68 458.
06 456.36
454.45 452.29 450.07 458.24 454.91 450.66 448.45 446.22 443.43 441.01 437.96 434.71 431.
31 427.58
416.96 431.14 435.60 439.12 443.85 448.26 451.10 454.10 455.72 457.90 459.58 460.75 462.
81 464.56
465.45 466.16 466.87 467.55 467.91"""
```

In [247]:
```
exp_envGC = GC.experimental_envelope(tGC, pGC, label=u"Gas Condensate- A.Shariati et al.
,2014")
```

In [248]:
```
for compound in GC.compounds:
    print compound.delta1
    print compound._get_eos_params('RKPR')
```

```
0.5
[ 2.30376808  0.0304338   0.5         1.54083759]
1.82758999
[ 14.61252217   0.07602789   1.82758999   2.11479414]
2.1325
[ 33.19203811   0.13055179   2.1325       2.62066497]
2.2395
[ 56.66096436   0.19214065   2.2395       3.11338964]
2.20390843
[ 95.67568042   0.29056435   2.20390843   3.6410622 ]
```

In [249]:
```
methane = GC.compounds [0]
methane.delta1 = 0.50
methane.save()

c4h10 = GC.compounds [1]
c4h10.delta1= 1.82758999
c4h10.save()

c7h16= GC.compounds [2]
c7h16.delta1= 2.13248282
c7h16.save()

c10h22= GC.compounds [3]
c10h22.delta1= 2.23953806
c10h22.save()

c14h30= GC.compounds [4]
c14h30.delta1= 2.20390843
c14h30.save()
```

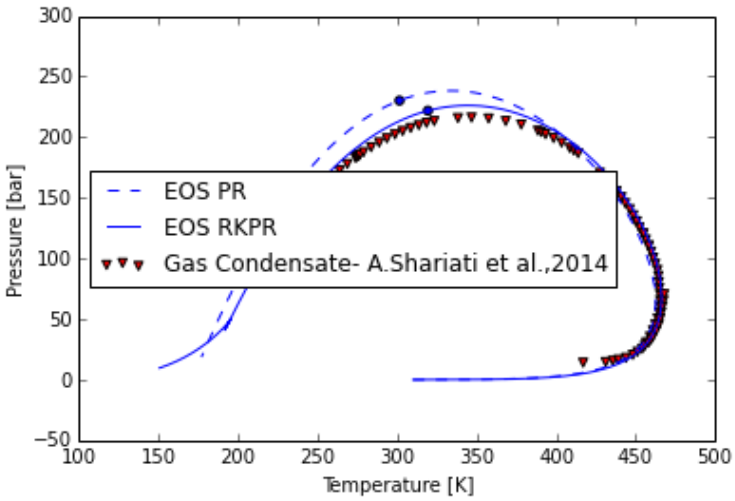
In [250]:
```
for compound in GC.compounds:
    print compound.delta1
    print compound._get_eos_params('RKPR')
```

```
0.5
[ 2.30376808  0.0304338   0.5         1.54083759]
1.82758999
[ 14.61252217   0.07602789   1.82758999   2.11479414]
2.13248282
[ 33.19200942   0.13055198   2.13248282   2.62066941]
2.23953806
[ 56.66107264   0.19214004   2.23953806   3.11337932]
2.20390843
[ 95.67568042   0.29056435   2.20390843   3.6410622 ]
```

In [251]:
```
setup_GC2 = EosSetup.objects.create(eos='RKPR', kij_mode=EosSetup.T_DEP,  lij_mode=EosSe
tup.CONSTANTS)

for c1, c2 in combinations(GC.compounds, 2):
    t = c1.tc if c1.weight < c2.weight else c2.tc
    setup_GC2.set_interaction('tstar', c1, c2, t)

setup_GC2.set_interaction('k0', 'methane', 'n-butane', 0.02177)
setup_GC2.set_interaction('k0', 'methane', 'n-heptane', 0.04678)
setup_GC2.set_interaction('k0', 'methane', 'n-decane', 0.06853)
setup_GC2.set_interaction('k0', 'methane', 'n-tetradecane', 0.08948)
setup_GC2.set_interaction('lij', 'methane', 'n-butane', -0.06565)
setup_GC2.set_interaction('lij', 'methane', 'n-heptane', -0.11875)
setup_GC2.set_interaction('lij', 'methane', 'n-decane', -0.14551)
setup_GC2.set_interaction('lij', 'methane', 'n-tetradecane', -0.13602)
setup_GC2.set_interaction('lij', 'n-butane', 'n-heptane', -0.01754)
setup_GC2.set_interaction('lij', 'n-butane', 'n-decane', -0.02433)
setup_GC2.set_interaction('lij', 'n-butane', 'n-tetradecane', -0.02203)
setup_GC2.set_interaction('lij', 'n-heptane', 'n-decane', -0.00586)
setup_GC2.set_interaction('lij', 'n-heptane', 'n-tetradecane', -0.00388)
setup_GC2.set_interaction('lij', 'n-decane', 'n-tetracosane', 0.00188)

envGC_RKPR= GC.get_envelope(setup_GC2, label=u"EOS RKPR")
```

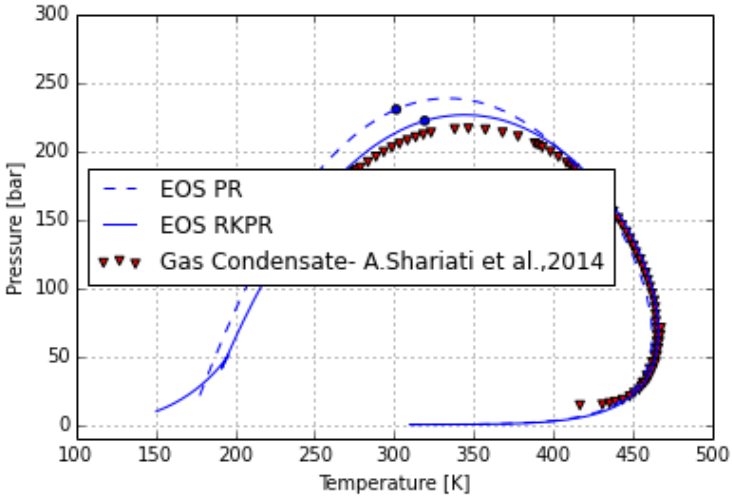
In [252]:
```
Caso_GyC= multiplot([envGC_PR, envGC_RKPR],[exp_envGC], formats=['--b','b'],experimental
_colors=['r'], experimental_markers=['v'], legends='best')
Caso_GyC
```

Out[252]:



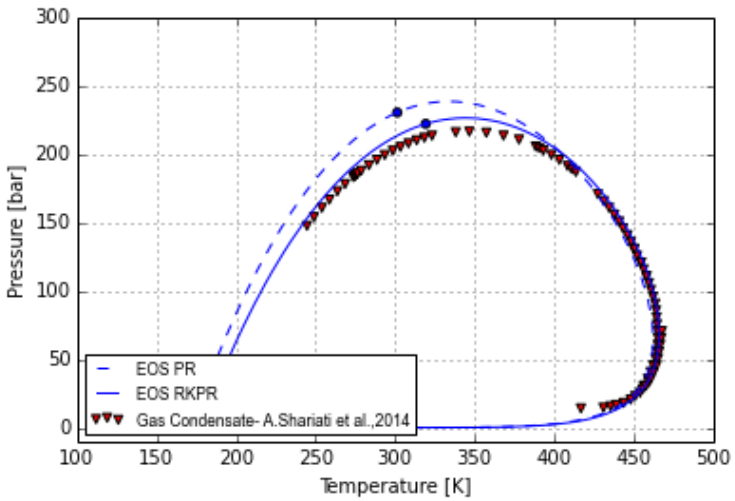
In [253]:
```
ax = Caso_GyC.gca()
ax.set_ylim([-10,300]),ax.grid(True)
Caso_GyC
```

Out[253]:



In [254]:
```
ax = Caso_GyC.get_axes()[0]

from matplotlib.font_manager import FontProperties

fontP = FontProperties()
fontP.set_size('small')
fontP.set_family('arial')
fontP.set_weight('normal')

ax.legend(loc='lower left', prop=fontP)
Caso_GyC
```

Out[254]:



In [255]:
```
Caso_GyC.savefig('Gas Condensate-A.Shariati_2014.jpg', dpi=600)
```

In [256]:
```
IP= Mixture()
```

In [257]:
```
IP.add_many("methane propane n-tetracosane", "0.7647 0.1501 0.0852")
```

In [258]:
```
IP.sort(True)
IP.compounds
```

Out[258]:
```
[<Compound: METHANE>, <Compound: PROPANE>, <Compound: n-TETRACOSANE>]
```

In [259]:
```
setup_IP1 = EosSetup.objects.create(eos='PR', kij_mode=EosSetup.CONSTANTS,  lij_mode=Eos
Setup.ZERO)
```

In [260]:
```
MatrizIP= """0 0.0167 0.0839
0 0 0.03
0 0 0"""
```

In [261]:
```
setup_IP1.set_interaction_matrix('kij', IP, MatrizIP)
```

In [262]:
```
envIP_PR= IP.get_envelope(setup_IP1, label=u"EOS PR")
envIP_PR
```

Out[262]:
```
<EosEnvelope: PR - kij constants - lij zero>
```

In [263]:
```
pIP= """627,4
626,4
623,4
620,4
618,4
615,4
609,4
599,4
590,3
577,3
565,3
554,3
543,3
532,3
520,3
508,3"""
```

In [264]:
```
tIP= """316,98
317,68
319,58
321,53
323,39
325,2
330,74
339,63
348,64
362,97
377,48
390,88
405,77
419,44
434,1
448,22"""
```

In [265]:
```
exp_envIP = IP.experimental_envelope(tIP, pIP, label=u"C1+C3+C24 Synthetic fluid by Flot
er et al.,1998")
```

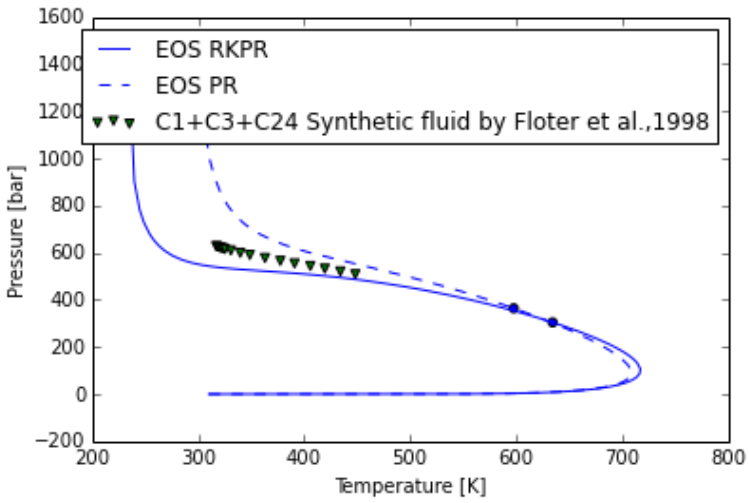
In [266]:
```
for compound in IP.compounds:
    print compound.delta1
    print compound._get_eos_params('RKPR')
```

```
0.5
[ 2.30376808  0.0304338   0.5         1.54083759]
1.6
[ 9.77170891  0.06017136  1.6         1.96439211]
1.8037
[ 202.2074408     0.55801882    1.8037        5.08757997]
```

In [267]:
```
setup_IP2=EosSetup.objects.create(eos='RKPR', kij_mode=EosSetup.T_DEP,  lij_mode=EosSetu
p.CONSTANTS)

for c1, c2 in combinations(IP.compounds, 2):
    t = c1.tc if c1.weight < c2.weight else c2.tc
    setup_IP2.set_interaction('tstar', c1, c2, t)

setup_IP2.set_interaction('k0', 'methane', 'propane', 0.01)
setup_IP2.set_interaction('k0', 'methane', 'n-tetracosane', 0.10717)
setup_IP2.set_interaction('lij', 'methane', 'propane', -0.04225)
setup_IP2.set_interaction('lij', 'methane', 'n-tetracosane', -0.06259)
setup_IP2.set_interaction('lij', 'propane', 'n-tetracosane', -0.01142)

envIP_RKPR= IP.get_envelope(setup_IP2, label=u"EOS RKPR")
```

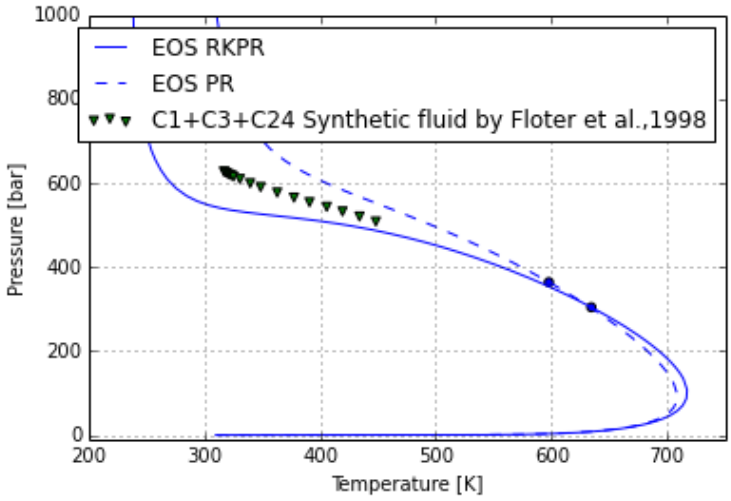
In [268]:
```
Caso_IP= multiplot([envIP_RKPR, envIP_PR],[exp_envIP],formats=['b','--b'], experimental_
colors=['g'], experimental_markers=['v'],legends='best')
Caso_IP
```

Out[268]:



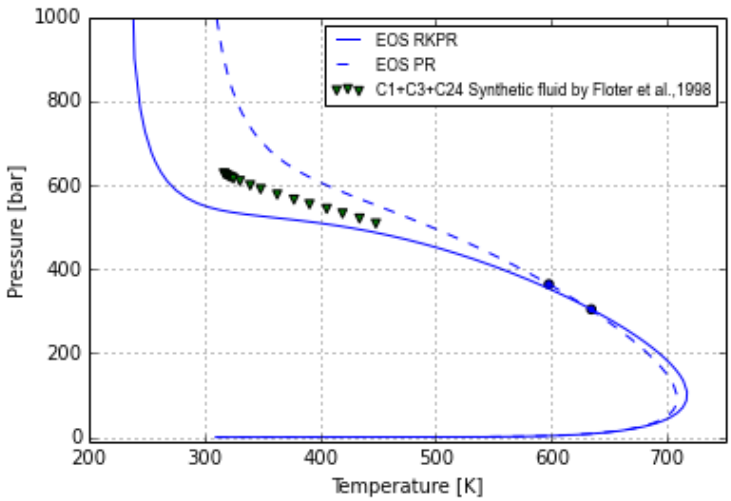
In [269]:
```
ax = Caso_IP.gca()
ax.set_ylim([-10,1000]),ax.grid(True)
ax.set_xlim([200,750])
Caso_IP
```

Out[269]:



In [270]:
```
ax = Caso_IP.get_axes()[0]

from matplotlib.font_manager import FontProperties

fontP = FontProperties()
fontP.set_size('small')
fontP.set_family('arial')
fontP.set_weight('normal')

ax.legend(loc='upper right', prop=fontP)
Caso_IP
```

Out[270]:



In [271]:
```
Caso_IP.savefig('Synthetic fluid by Floter_1998.jpg', dpi=600)
```

In [272]:
```
IV = Mixture()
```

In [273]:
```
elementos= ['nitrogen', 'carbon dioxide', 'methane', 'ethane', 'propane', 'n-butane', 'n
-pentane', 'n-hexane', 'n-heptane', 'n-octane', 'n-nonane']
```

In [274]:
```
fracciones= [0.0067, 0.004, 0.77751, 0.10507, 0.08257, 0.00992, 0.00774, 0.00318, 0.0019
6, 0.00105, 0.0003]
```

In [275]:
```
for elemento, fraccion in zip(elementos, fracciones):
    IV[elemento]= fraccion
```

In [276]:
```
IV
```

Out[276]:
```
[(<Compound: NITROGEN>, Decimal('0.0067')), (<Compound: CARBON DIOXIDE>, Decimal('0.004'
)), (<Compound: METHANE>, Decimal('0.77751')), (<Compound: ETHANE>, Decimal('0.10507')),
 (<Compound: PROPANE>, Decimal('0.08257')), (<Compound: n-BUTANE>, Decimal('0.00992')),
(<Compound: n-PENTANE>, Decimal('0.00774')), (<Compound: n-HEXANE>, Decimal('0.00318')),
 (<Compound: n-HEPTANE>, Decimal('0.00196')), (<Compound: n-OCTANE>, Decimal('0.00105'))
, (<Compound: n-NONANE>, Decimal('0.0003'))]
```

In [277]:
```
IV.sort(True)
```

In [278]:
```
IV
```

Out[278]:
```
[(<Compound: METHANE>, Decimal('0.77751')), (<Compound: NITROGEN>, Decimal('0.0067')), (
<Compound: ETHANE>, Decimal('0.10507')), (<Compound: CARBON DIOXIDE>, Decimal('0.004')),
 (<Compound: PROPANE>, Decimal('0.08257')), (<Compound: n-BUTANE>, Decimal('0.00992')),
(<Compound: n-PENTANE>, Decimal('0.00774')), (<Compound: n-HEXANE>, Decimal('0.00318')),
 (<Compound: n-HEPTANE>, Decimal('0.00196')), (<Compound: n-OCTANE>, Decimal('0.00105'))
, (<Compound: n-NONANE>, Decimal('0.0003'))]
```

In [279]:
```
setup_IV1 = EosSetup.objects.create(eos='PR', kij_mode=EosSetup.CONSTANTS,  lij_mode=Eos
Setup.ZERO)
```

In [280]:
```
matrizIV= """0 0,0242 0,0114 0,0884 0,0167 0,0218 0,0265 0,0311 0,0354 0,0396 0,0435
0 0 0,0587 -0,0225 0,0855 0,1064 0,1227 0,1354 0,1452 0,1529 0,1589
0 0 0 0,1184 0 0 0 0 0 0 0
0 0 0 0 0,1338 0,1417 0,1457 0,1478 0,1489 0,1494 0,1497
0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0"""
```

In [281]:
```
setup_IV1.set_interaction_matrix('kij', IV, matrizIV)
```

In [282]:
```
envIV_PR = IV.get_envelope(setup_IV1,label=u"EOS PR")
```

In [283]:
```
pIV= """35,7
72,42
93,48
108,56
114,25
114,49
111,66"""
```

In [284]:
```
tIV= """325,1
322,5
313,9
302,1
286,5
275,5
264,5"""
```

In [285]:
```
exp_envIV = IV.experimental_envelope(tIV, pIV, label=u"Wet Natural Gas-M.Atilhan et al.,
2010")
```

In [286]:
```
c5h12= IV.compounds [6]
c5h12.delta1= 1.95731509
c5h12.save()

c6h14= IV.compounds [7]
c6h14.delta1= 2.05756499
c6h14.save()

c7h16= IV.compounds [8]
c7h16.delta1= 2.13248282
c7h16.save()

c8h18= IV.compounds [9]
c8h18.delta1= 2.18571421
c8h18.save()

c9h20= IV.compounds [10]
c9h20.delta1= 2.22046251
c9h20.save()
```

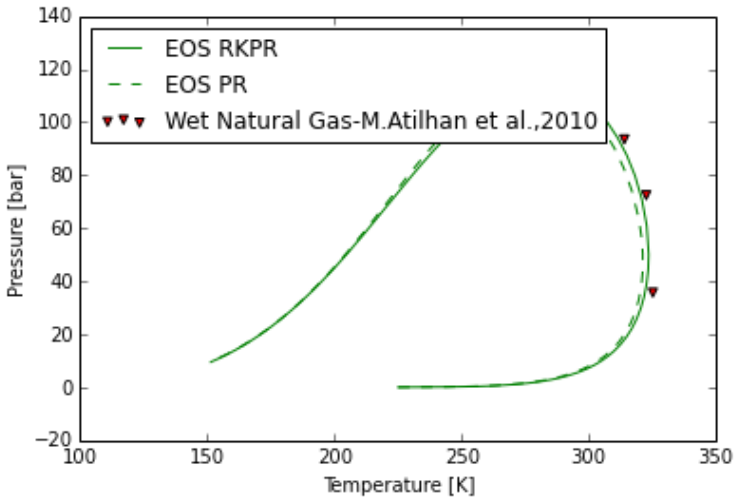
In [287]:
```
for compound in IV.compounds:
    print compound.delta1
    print compound._get_eos_params('RKPR')
```

```
0.5
[ 2.30376808  0.0304338   0.5         1.54083759]
None
[ 1.37713479  0.02694987  0.85180012  1.62485788]
0.8
[ 5.61628283  0.04561112  0.8         1.90385075]
None
[ 3.85211219  0.02791465  1.85325193  2.20290185]
1.6
[ 9.77170891  0.06017136  1.6         1.96439211]
1.82758999
[ 14.61252217   0.07602789   1.82758999   2.11479414]
1.95731509
[ 20.22369723   0.09363098   1.95731509   2.28798762]
2.05756499
[ 26.44574674   0.11180452   2.05756499   2.45650771]
2.13248282
[ 33.19200942   0.13055198   2.13248282   2.62066941]
2.18571421
[ 40.58865788   0.15057346   2.18571421   2.79307492]
2.22046251
[ 48.32927702   0.17068719   2.22046251   2.94387153]
```

In [288]:
```
setup_IV2= EosSetup.objects.create(eos='RKPR', kij_mode=EosSetup.T_DEP,  lij_mode=EosSet
up.CONSTANTS)

for c1, c2 in combinations(IV.compounds, 2):
    t = c1.tc if c1.weight < c2.weight else c2.tc
    setup_IV2.set_interaction('tstar', c1, c2, t)

setup_IV2.set_interaction('k0', 'methane', 'ethane', 0.00307)
setup_IV2.set_interaction('k0', 'methane', 'propane', 0.01)
setup_IV2.set_interaction('k0', 'methane', 'n-butane', 0.02177)
setup_IV2.set_interaction('k0', 'methane', 'n-pentane', 0.03022)
setup_IV2.set_interaction('k0', 'methane', 'n-hexane', 0.03864)
setup_IV2.set_interaction('k0', 'methane', 'n-heptane', 0.04678)
setup_IV2.set_interaction('k0', 'methane', 'n-octane', 0.05464)
setup_IV2.set_interaction('k0', 'methane', 'n-nonane', 0.06183)

setup_IV2.set_interaction('lij', 'methane', 'ethane', -0.0079)
setup_IV2.set_interaction('lij', 'methane', 'propane', -0.04225)
setup_IV2.set_interaction('lij', 'methane', 'n-butane', -0.06565)
setup_IV2.set_interaction('lij', 'methane', 'n-pentane', -0.08473)
setup_IV2.set_interaction('lij', 'methane', 'n-hexane', -0.10288)
setup_IV2.set_interaction('lij', 'methane', 'n-heptane', -0.11875)
setup_IV2.set_interaction('lij', 'methane', 'n-octane', -0.13141)
setup_IV2.set_interaction('lij', 'methane', 'n-nonane', -0.14036)
setup_IV2.set_interaction('lij', 'ethane', 'propane', -0.0105)
setup_IV2.set_interaction('lij', 'ethane', 'n-butane', -0.00437)
setup_IV2.set_interaction('lij', 'ethane', 'n-pentane', -0.00616)
setup_IV2.set_interaction('lij', 'ethane', 'n-hexane', -0.00798)
setup_IV2.set_interaction('lij', 'ethane', 'n-heptane', -0.00967)
setup_IV2.set_interaction('lij', 'ethane', 'n-octane', -0.01108)
setup_IV2.set_interaction('lij', 'ethane', 'n-nonane', -0.0121)
setup_IV2.set_interaction('lij', 'propane', 'n-butane', -0.01284)
setup_IV2.set_interaction('lij', 'propane', 'n-pentane', -0.02082)
setup_IV2.set_interaction('lij', 'propane', 'n-hexane', -0.02734)
setup_IV2.set_interaction('lij', 'propane', 'n-heptane', -0.03242)
setup_IV2.set_interaction('lij', 'propane', 'n-octane', -0.03614)
setup_IV2.set_interaction('lij', 'propane', 'n-nonane', -0.03862)
setup_IV2.set_interaction('lij', 'n-butane', 'n-pentane', -0.00714)
setup_IV2.set_interaction('lij', 'n-butane', 'n-hexane', -0.01298)
setup_IV2.set_interaction('lij', 'n-butane', 'n-heptane', -0.01754)
setup_IV2.set_interaction('lij', 'n-butane', 'n-octane', -0.02087)
setup_IV2.set_interaction('lij', 'n-butane', 'n-nonane', -0.0231)
setup_IV2.set_interaction('lij', 'n-pentane', 'n-hexane', -0.00548)
setup_IV2.set_interaction('lij', 'n-pentane', 'n-heptane', -0.00976)
setup_IV2.set_interaction('lij', 'n-pentane', 'n-octane', -0.01289)
setup_IV2.set_interaction('lij', 'n-pentane', 'n-nonane', -0.01498)
setup_IV2.set_interaction('lij', 'n-hexane', 'n-heptane', -0.00407)
setup_IV2.set_interaction('lij', 'n-hexane', 'n-octane', -0.00705)
setup_IV2.set_interaction('lij', 'n-hexane', 'n-nonane', -0.00905)
setup_IV2.set_interaction('lij', 'n-heptane', 'n-octane', -0.00287)
setup_IV2.set_interaction('lij', 'n-heptane', 'n-nonane', -0.00479)
setup_IV2.set_interaction('lij', 'n-octane', 'n-nonane', -0.00187)
```

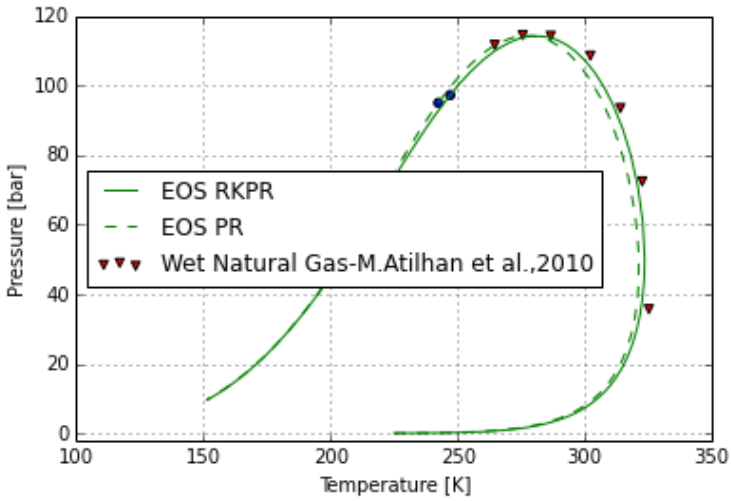
In [289]:
```
Caso_IV= multiplot([envIV_RKPR, envIV_PR],[exp_envIV], formats=['-g','--g'], experimenta
l_colors=['r'], experimental_markers=['v'], legends='best')
Caso_IV
```

Out[289]:



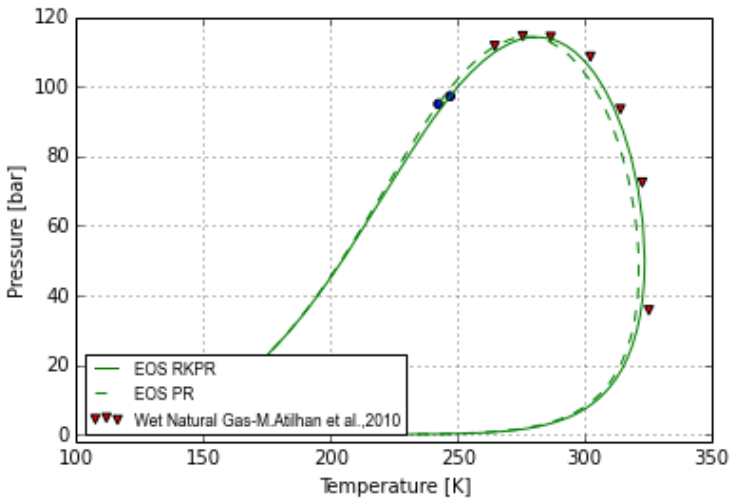
In [290]:
```
ax = Caso_IV.gca()
ax.set_ylim([-2,120]),ax.grid(True)
Caso_IV
```

Out[290]:



In [291]:
```
ax = Caso_IV.get_axes()[0]

from matplotlib.font_manager import FontProperties

fontP = FontProperties()
fontP.set_size('small')
fontP.set_family('arial')
fontP.set_weight('normal')

ax.legend(loc='lower left', prop=fontP)
Caso_IV
```

Out[291]:



In [292]:
```
Caso_IV.savefig('Wet Natural Gas-Atilhan_2010.jpg', dpi=600)
```

In [293]:
```
GN = Mixture()
```

In [294]:
```
GN.add_many("methane ethane propane isobutane n-butane benzene", "0.84080 0.09973 0.0403
7 0.00603 0.01012 0,002959")
```

In [295]:
```
GN
```

Out[295]:
```
[(<Compound: METHANE>, Decimal('0.8408')), (<Compound: ETHANE>, Decimal('0.09973')), (<C
ompound: PROPANE>, Decimal('0.04037')), (<Compound: ISOBUTANE>, Decimal('0.00603')), (<C
ompound: n-BUTANE>, Decimal('0.01012')), (<Compound: BENZENE>, Decimal('0.00295'))]
```

In [296]:
```
setup_GN1 = EosSetup.objects.create(eos='PR', kij_mode=EosSetup.CONSTANTS,  lij_mode=Eos
Setup.ZERO)
```

In [297]:
```
matrizGN = """0 0.0114 0.0167 0.0218 0.0218 0
0 0 0.0011 0.0096 0.0096 0
0 0 0 0.0033 0.0033 0
0 0 0 0 0 0
0 0 0 0 0 0
0 0 0 0 0 0"""
```

In [298]:
```
setup_GN1.set_interaction_matrix('kij', GN, matrizGN)
```

In [299]:
```
envGN_PR= GN.get_envelope(setup_GN1, label=u"EOS PR")
envGN_PR
```

Out[299]:
```
<EosEnvelope: PR - kij constants - lij zero>
```

In [300]:
```
pGN= """95,5
94,4
93,2
92
90,8
88,7
85,7
82
79,4
76
73,1
68,2
64,8
60,1
55,5
53
47,2
41,6
37
32
27,6
22,4
16,9
14
12,1
8,8
5,4
2,9"""
```

In [301]:
```
tGN= """259,4
261,1
262,9
264,2
265,5
266,8
268,6
270,5
271,4
273
273,6
275,1
276
276,4
276,7
277,1
277,3
277,3
276,9
276,2
275,2
273,7
271,4
269,4
268,1
264,9
260
255,2"""
```

In [302]:
```
exp_envGN = GN.experimental_envelope(tGN, pGN, label=u"Natural Gas-V.Louli et al.,2012")
```

In [303]:
```
methane = GN.compounds [0]
methane.delta1 = 0.50
methane.save()

c2h6= GN.compounds [1]
c2h6.delta1= 0.8
c2h6.save()

c3h8= GN.compounds [2]
c3h8.delta1= 1.60
c3h8.save()

isobutane=GN.compounds [3]
isobutane.delta1= 1.70
isobutane.save()

c4h10=GN.compounds [4]
c4h10.delta1= 1.82758999
c4h10.save()
```

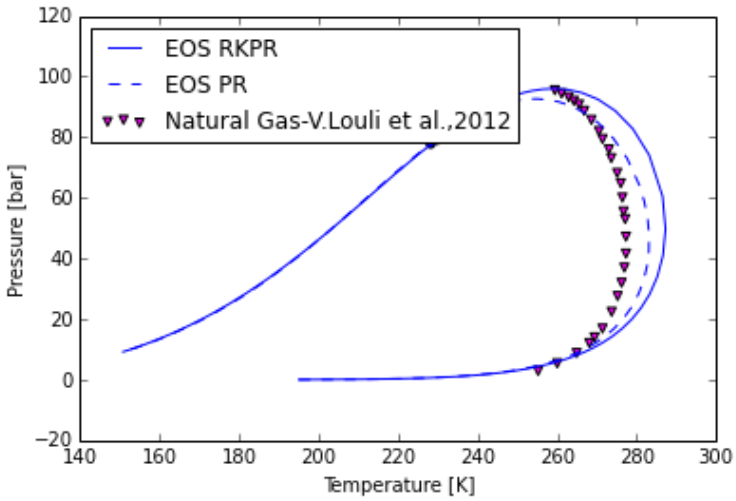
In [304]:
```
for compound in GN.compounds:
    print compound.delta1
    print compound._get_eos_params('RKPR')
```

```
0.5
[ 2.30376808  0.0304338   0.5         1.54083759]
0.8
[ 5.61628283  0.04561112  0.8         1.90385075]
1.6
[ 9.77170891  0.06017136  1.6         1.96439211]
1.7
[ 13.93386133   0.07683114   1.7          2.07758116]
1.82758999
[ 14.61252217   0.07602789   1.82758999   2.11479414]
None
[ 20.20708826   0.07544854   2.22553038   2.05873355]
```

In [305]:
```
setup_GN2 = EosSetup.objects.create(eos='RKPR', kij_mode=EosSetup.T_DEP,  lij_mode=EosSe
tup.CONSTANTS)

for c1, c2 in combinations(GN.compounds, 2):
    t = c1.tc if c1.weight < c2.weight else c2.tc
    setup_GN2.set_interaction('tstar', c1, c2, t)

setup_GN2.set_interaction('k0', 'methane', 'ethane', 0.00307)
setup_GN2.set_interaction('k0', 'methane', 'propane', 0.01)
setup_GN2.set_interaction('k0', 'methane', 'isobutane', 0.02177)
setup_GN2.set_interaction('k0', 'methane', 'n-butane', 0.02177)

setup_GN2.set_interaction('lij', 'methane', 'ethane', -0.0079)
setup_GN2.set_interaction('lij', 'methane', 'propane', -0.04225)
setup_GN2.set_interaction('lij', 'methane', 'isobutane', -0.06565)
setup_GN2.set_interaction('lij', 'methane', 'n-butane', -0.06565)
setup_GN2.set_interaction('lij', 'ethane', 'propane', -0.0105)
setup_GN2.set_interaction('lij', 'ethane', 'isobutane', -0.00437)
setup_GN2.set_interaction('lij', 'ethane', 'n-butane', -0.00437)
setup_GN2.set_interaction('lij', 'propane', 'isobutane', -0.01284)
setup_GN2.set_interaction('lij', 'propane', 'n-butane', -0.01284)

envGN_RKPR= GN.get_envelope(setup_GN2, label=u"EOS RKPR")
```

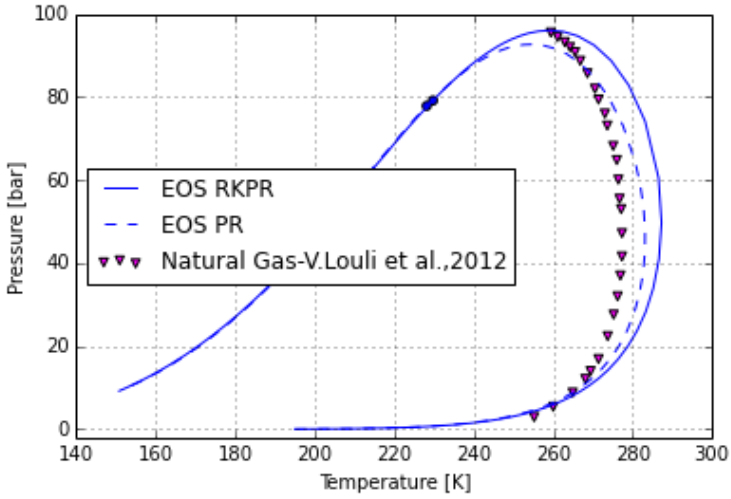
In [306]:
```
Caso_GN= multiplot([envGN_RKPR, envGN_PR],[exp_envGN], formats=['b','--b'], experimental
_colors=['magenta'], experimental_markers=['v'],legends='best')
Caso_GN
```

Out[306]:



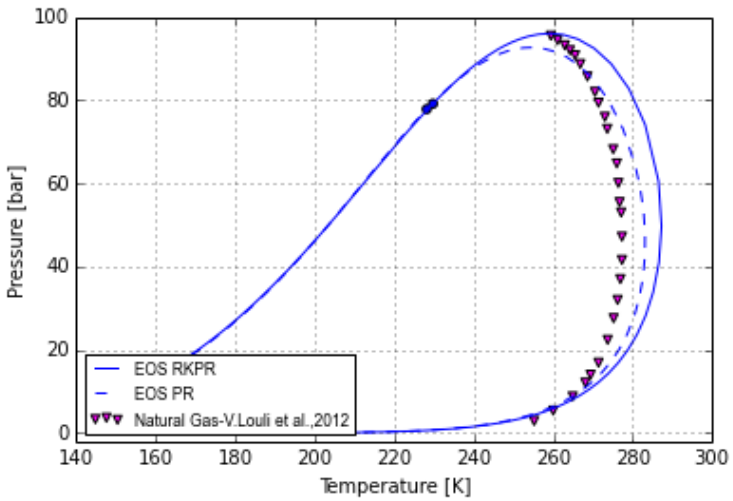
In [307]:
```
ax = Caso_GN.gca()

ax.set_ylim([-2,100]),ax.grid(True)

Caso_GN
```

Out[307]:



In [308]:
```
ax = Caso_GN.get_axes()[0]

from matplotlib.font_manager import FontProperties

fontP = FontProperties()
fontP.set_size('small')
fontP.set_family('arial')
fontP.set_weight('normal')

ax.legend(loc='lower left', prop=fontP)
Caso_GN
```

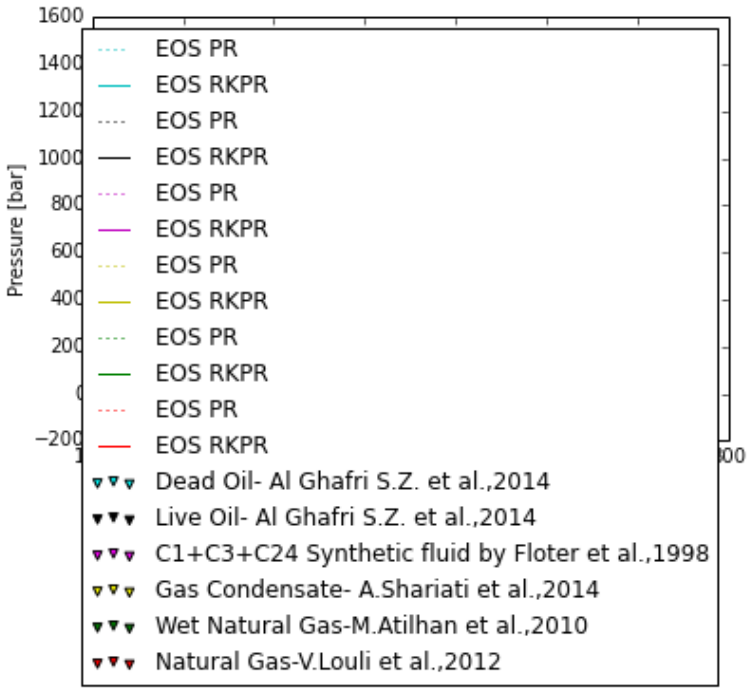
Out[308]:



In [309]:
```
Caso_GN.savefig('Natural Gas-Louli_2012.jpg', dpi=600)
```

In [310]:
```
figuratotal= multiplot([envP_PR,envP_RKPR,envLiveOil_PR, envLiveOil_RKPR, envIP_PR,envIP
_RKPR,envGC_PR,envGC_RKPR,envIV_PR,envIV_RKPR,envGN_PR,envGN_RKPR],[exp_envP,exp_envLive
Oil, exp_envIP,exp_envGC,exp_envIV,exp_envGN], formats=[':c','c',':k','k',':m','m',':y',
'y',':g','g',':r','r'],experimental_colors=['cyan','black','magenta', 'yellow','green','
red'], experimental_markers= ['v','v','v','v','v','v'],legends='upper right')

figuratotal
```

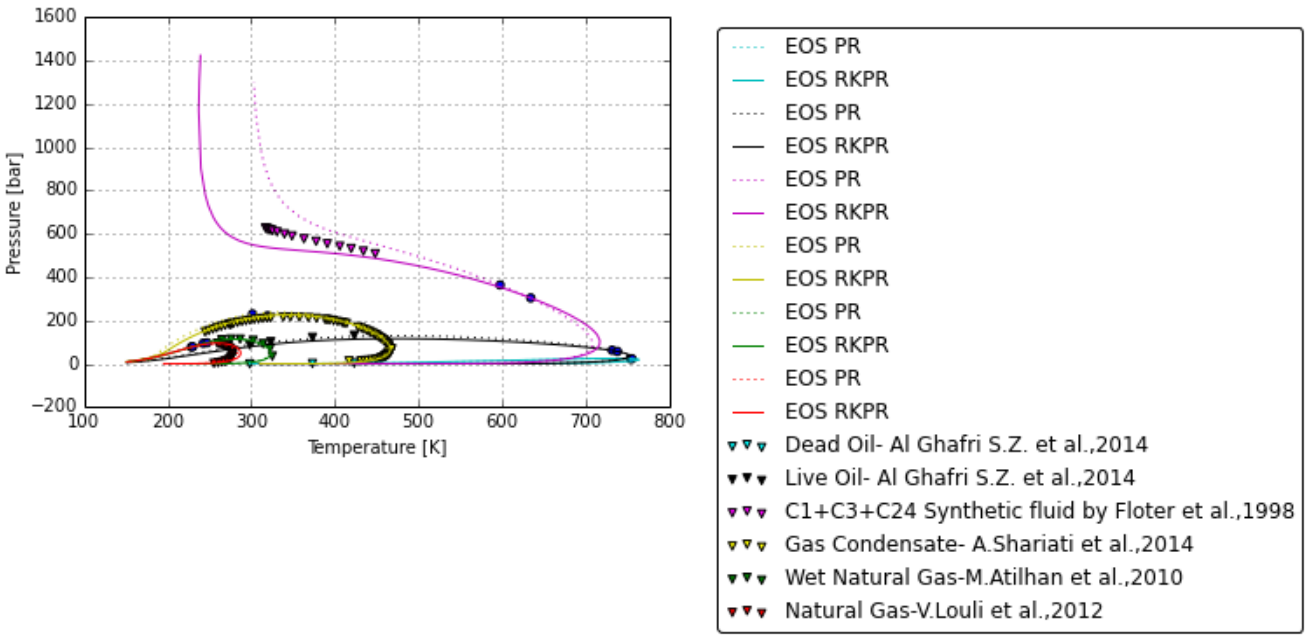
Out[310]:



In [311]:
```
figuratotal.savefig('leyenda de todos.jpg',dpi=1200)
```

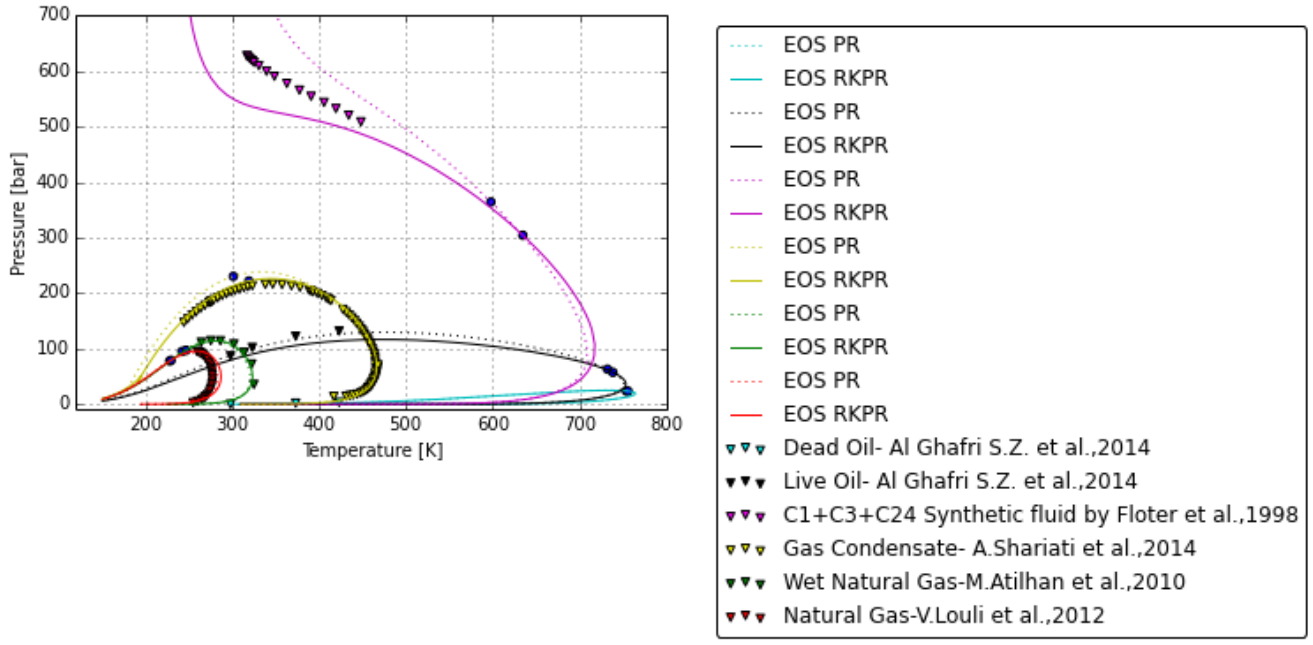
In [312]:
```
ax = figuratotal.get_axes()[0]
ax.legend(bbox_to_anchor=(2.1,1),fancybox=True)
figuratotal
```

Out[312]:



In [313]:
```
ax = figuratotal.gca()
ax.set_ylim([-10,700]),ax.grid(True)
ax.set_xlim([120,800])
figuratotal
```

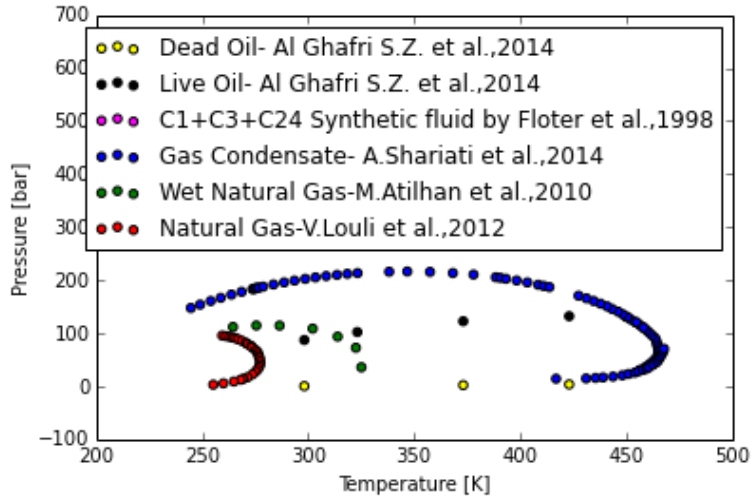
Out[313]:



In [314]:
```
figuratotal.savefig('clasificacion fluidos sinteticos final.jpg', dpi=1200)
```

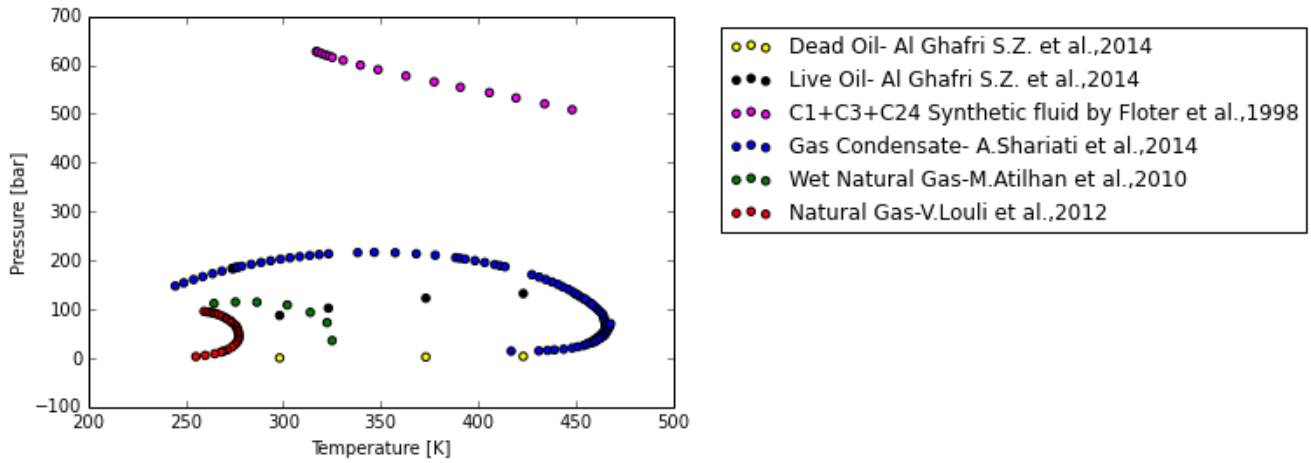
In [315]:
```
figuraexp= multiplot(None, [exp_envP,exp_envLiveOil,exp_envIP,exp_envGC,exp_envIV,exp_en
vGN],experimental_colors=['yellow','black','magenta','blue','green','red'],experimental_
markers=['o','o','o','o','o','o'],legends='upper right')
figuraexp
```

Out[315]:



In [316]:
```
ax = figuraexp.get_axes()[0]
ax.legend(loc='upper right',bbox_to_anchor=(2.1,1))
figuraexp
```

Out[316]:

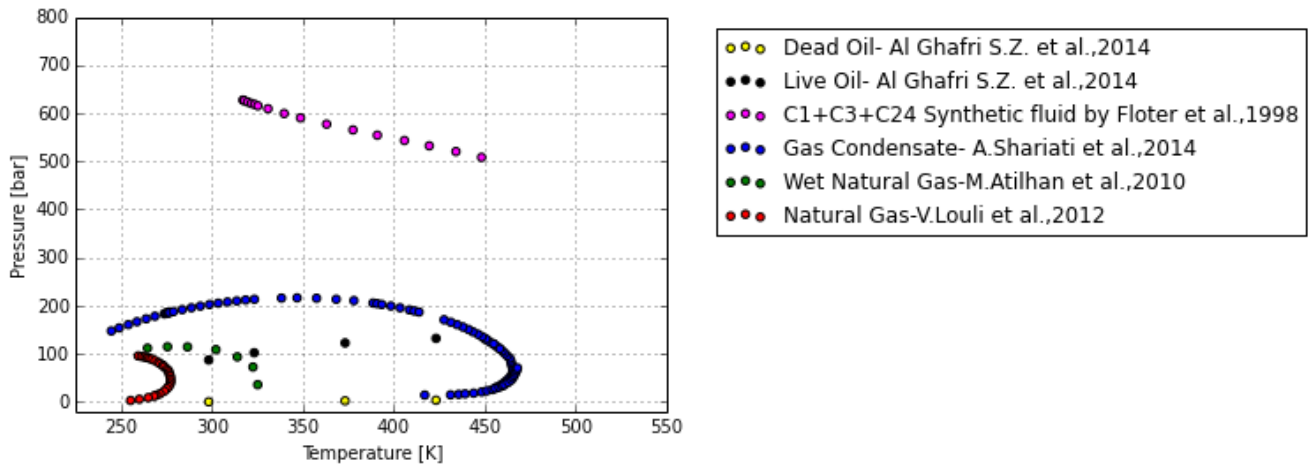


In [317]:
```
ax = figuraexp.gca()
ax.set_ylim([-20,800]),ax.grid(True)
```

Out[317]:
```
((-20, 800), None)
```

In [318]:
```
ax.set_xlim([225,550])
figuraexp
```

Out[318]:



In [319]:
```
figuraexp.savefig('grafico experimental final.jpg', dpi=900)
```

In [319]:
```
```