Propyne

Other names:	1-Propyne
	Acetylene, methyl-
	Allylene
	CH3C«equiv»CH
	CH3CÂ«equivÂ»CH
	Methylacetylene
	Propine
Inchi:	InChI=1S/C3H4/c1-3-2/h1H,2H3
InchiKey:	MWWATHDPGQKSAR-UHFFFAOYSA-N
Formula:	C3H4
SMILES:	C#CC
Mol. weight [g/mol]:	40.06
CAS:	74-99-7

Physical Properties

Property code	Value	Unit	Source
af	0.2150		KDB
affp	748.00	kJ/mol	NIST Webbook
basg	723.00	kJ/mol	NIST Webbook
dm	0.70	debye	KDB
gf	194.60	kJ/mol	KDB
hcg	1924.64	kJ/mol	KDB
hcn	1832.592	kJ/mol	KDB
hf	185.60	kJ/mol	KDB
hf	185.40 ± 0.88	kJ/mol	NIST Webbook
hfus	6.50	kJ/mol	Joback Method
hvap	22.13	kJ/mol	Joback Method
ie	10.50 ± 0.10	eV	NIST Webbook
ie	10.37	eV	NIST Webbook
ie	10.36 ± 0.01	eV	NIST Webbook
ie	10.36	eV	NIST Webbook
ie	10.54	eV	NIST Webbook
ie	10.37 ± 0.01	eV	NIST Webbook
ie	10.38 ± 0.02	eV	NIST Webbook
ie	10.36 ± 0.02	eV	NIST Webbook
ie	10.35 ± 0.01	eV	NIST Webbook
ie	10.37	eV	NIST Webbook

ie	10.37 ± 0.01	eV	NIST Webbook
ie	10.36	eV	NIST Webbook
ie	10.36	eV	NIST Webbook
ie	10.36 ± 0.01	eV	NIST Webbook
ie	10.37 ± 0.02	eV	NIST Webbook
ie	10.38 ± 0.01	eV	NIST Webbook
ie	10.37 ± 0.01	eV	NIST Webbook
ie	10.37	eV	NIST Webbook
ie	10.36 ± 0.01	eV	NIST Webbook
ie	10.37	eV	NIST Webbook
log10ws	-0.41		Estimated Solubility Method
logp	0.639		Crippen Method
mcvol	44.530	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	5630.00 ± 20.00	kPa	NIST Webbook
pc	5630.00	kPa	KDB
pc	5627.59 ± 5.06	kPa	NIST Webbook
rhoc	245.19 ± 0.80	kg/m3	NIST Webbook
rhoc	244.91 ± 0.40	kg/m3	NIST Webbook
rinpol	334.00		NIST Webbook
rinpol	330.00		NIST Webbook
rinpol	299.00		NIST Webbook
rinpol	339.00		NIST Webbook
rinpol	340.00		NIST Webbook
rinpol	311.00		NIST Webbook
rinpol	316.00		NIST Webbook
rinpol	297.00		NIST Webbook
rinpol	299.00		NIST Webbook
rinpol	328.00		NIST Webbook
rinpol	339.00		NIST Webbook
rinpol	323.60		NIST Webbook
tb	244.70 ± 0.30	K	NIST Webbook
tb	249.65 ± 0.50	K	NIST Webbook
tb	249.90 ± 0.30	K	NIST Webbook
tb	250.15 ± 1.50	K	NIST Webbook
tb	249.85 ± 1.00	K	NIST Webbook
tb	249.95 ± 1.00	K	NIST Webbook
tb	250.00	K	NIST Webbook
tb	249.90	K	NIST Webbook
tb	249.90	K	KDB
tb	250.45 ± 1.00	K	NIST Webbook
tb	249.35 ± 0.50	K	NIST Webbook

tb	250.15 ± 1.00	K	NIST Webbook
tb	250.00 ± 1.00	K	NIST Webbook
tb	249.92 ± 0.10	K	NIST Webbook
tb	249.93 ± 0.30	K	NIST Webbook
tb	249.93 ± 0.20	K	NIST Webbook
tb	249.95 ± 0.50	K	NIST Webbook
tb	250.65 ± 1.50	K	NIST Webbook
tb	249.93 ± 0.30	K	NIST Webbook
tb	249.93 ± 0.20	K	NIST Webbook
tc	402.38 ± 0.05	K	NIST Webbook
tc	402.40 ± 0.20	K	NIST Webbook
tc	401.10 ± 0.50	K	NIST Webbook
tc	402.40	K	KDB
tf	170.40	K	KDB
tt	168.50 ± 0.30	K	NIST Webbook
vc	0.164	m3/kmol	NIST Webbook
vc	0.164	m3/kmol	KDB
zc	0.2751260		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	65.10	J/mol×K	332.83	NIST Webbook
cpg	69.12	J/mol×K	369.21	NIST Webbook
cpg	57.57	J/mol×K	272.28	NIST Webbook
cpg	61.00	J/mol×K	299.59	NIST Webbook
hvapt	21.40	kJ/mol	230.00	NIST Webbook
hvapt	23.40	kJ/mol	222.00	NIST Webbook
hvapt	22.13	kJ/mol	249.80	KDB
hvapt	23.00	kJ/mol	220.00	NIST Webbook
hvapt	20.80	kJ/mol	329.50	NIST Webbook
hvapt	21.20	kJ/mol	332.00	NIST Webbook
hvapt	21.90	kJ/mol	380.50	NIST Webbook
hvapt	23.20	kJ/mol	277.50	NIST Webbook
hvapt	22.10	kJ/mol	275.00	NIST Webbook
hvapt	23.90	kJ/mol	208.50	NIST Webbook
hvapt	21.60	kJ/mol	361.50	NIST Webbook
rhol	706.00	kg/m3	223.00	KDB
srf	0.02	N/m	203.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44642e+01
Coeff. B	-2.12600e+03
Coeff. C	-3.20710e+01
Temperature range (K), min.	170.50
Temperature range (K), max.	402.38

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.57423e+01
Coeff. B	-4.40094e+03
Coeff. C	-8.01385e+00
Coeff. D	1.16420e-05
Temperature range (K), min.	170.45
Temperature range (K), max.	402.39

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74997&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=400

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=400

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter