Allene

Other names:	1,2-Propadiene
	CH2=C=CH2
	DIMETHYLENEMETHANE
	PROPA-1,2-DIENE
	Propadiene
	sym-Allylene
Inchi:	InChI=1S/C3H4/c1-3-2/h1-2H2
InchiKey:	IYABWNGZIDDRAK-UHFFFAOYSA-N
Formula:	C3H4
SMILES:	C=C=C
Mol. weight [g/mol]:	40.06
CAS:	463-49-0

Physical Properties

Property code	Value	Unit	Source
af	0.3130		KDB
affp	775.30	kJ/mol	NIST Webbook
basg	745.80	kJ/mol	NIST Webbook
dm	0.20	debye	KDB
gf	202.50	kJ/mol	KDB
hcg	1928.82	kJ/mol	KDB
hcn	1840.960	kJ/mol	KDB
hf	192.30	kJ/mol	KDB
hfus	2.89	kJ/mol	Joback Method
hvap	21.41	kJ/mol	Joback Method
ie	10.02	eV	NIST Webbook
ie	9.62 ± 0.04	eV	NIST Webbook
ie	10.07	eV	NIST Webbook
ie	9.83	eV	NIST Webbook
ie	9.53 ± 0.03	eV	NIST Webbook
ie	9.69 ± 0.00	eV	NIST Webbook
ie	9.62	eV	NIST Webbook
ie	9.62 ± 0.02	eV	NIST Webbook
ie	10.20 ± 0.10	eV	NIST Webbook
ie	9.69 ± 0.00	eV	NIST Webbook
ie	10.02 ± 0.00	eV	NIST Webbook
ie	10.06	eV	NIST Webbook

ie	9.69 ± 0.00	eV	NIST Webbook
ie	9.70 ± 0.00	eV	NIST Webbook
ie	9.69	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
log10ws	-0.81		Crippen Method
logp	0.957		Crippen Method
mcvol	44.530	ml/mol	McGowan Method
pc	5250.00	kPa	NIST Webbook
pc	5250.00	kPa	KDB
rinpol	316.00		NIST Webbook
rinpol	311.00		NIST Webbook
rinpol	329.50		NIST Webbook
rinpol	317.00		NIST Webbook
rinpol	326.00		NIST Webbook
rinpol	337.00		NIST Webbook
rinpol	320.00		NIST Webbook
rinpol	336.00		NIST Webbook
rinpol	326.00		NIST Webbook
rinpol	318.00		NIST Webbook
rinpol	319.00		NIST Webbook
tb	238.00 ± 2.00	K	NIST Webbook
tb	238.85 ± 1.00	K	NIST Webbook
tb	238.70	K	KDB
tb	241.00	K	NIST Webbook
tb	241.00 ± 4.00	K	NIST Webbook
tb	241.00 ± 3.00	K	NIST Webbook
tb	239.51 ± 1.00	K	NIST Webbook
tb	238.65 ± 0.40	K	NIST Webbook
tc	394.00	K	KDB
tc	394.00	K	NIST Webbook
tf	127.00 ± 10.00	K	NIST Webbook
tf	136.87	K	KDB
tf	137.10 ± 0.30	K	NIST Webbook
tt	136.59 ± 0.20	K	NIST Webbook
vc	0.162	m3/kmol	KDB
zc	0.2596220		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	63.81 ± 0.26	J/mol×K	334.00	NIST Webbook
cpg	67.86 ± 0.27	J/mol×K	366.45	NIST Webbook
cpg	40.63 ± 0.16	J/mol×K	148.20	NIST Webbook
cpg	41.49 ± 0.17	J/mol×K	157.80	NIST Webbook
cpg	47.53 ± 0.19	J/mol×K	213.10	NIST Webbook
cpg	48.30 ± 0.19	J/mol×K	218.40	NIST Webbook
cpg	49.02 ± 0.20	J/mol×K	223.70	NIST Webbook
cpg	53.31 ± 0.21	J/mol×K	258.00	NIST Webbook
cpg	55.23 ± 0.22	J/mol×K	272.16	NIST Webbook
cpg	59.33 ± 0.24	J/mol×K	300.00	NIST Webbook
hvapt	21.50	kJ/mol	230.00	NIST Webbook
hvapt	20.90	kJ/mol	219.50	NIST Webbook
hvapt	18.62	kJ/mol	241.20	KDB
hvapt	22.60	kJ/mol	205.00	NIST Webbook
hvapt	19.90	kJ/mol	219.50	NIST Webbook
hvapt	21.30	kJ/mol	195.50	NIST Webbook
hvapt	22.90	kJ/mol	163.50	NIST Webbook
rhol	658.00	kg/m3	238.00	KDB
srf	0.02	N/m	233.20	KDB

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C463490&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol356.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
pc:	Critical Pressure
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