1-Buten-3-yne, 2-methyl-

Other names:	Isopropenylacetylene
	CH2=C(CH3)C«equiv»CH
	2-Methyl-1-buten-3-yne
	2-Methylbut-1-en-3-yne
	Valylene
	3-Methyl-3-buten-1-yne
	2-Methylbutenyne
	2-Methyl-1-butenyne
	1-Butene-3-yne, 2-methyl-
	NSC 9296
	3-Methyl-3-butene-1-yne
Inchi:	InChI=1S/C5H6/c1-4-5(2)3/h1H,2H2,3H3
InchiKey:	BOFLDKIFLIFLJA-UHFFFAOYSA-N
Formula:	C5H6
SMILES:	C#CC(=C)C
Mol. weight [g/mol]:	66.10
CAS:	78-80-8

Physical Properties

Property code	Value	Unit	Source
chl	-3056.00 ± 0.80	kJ/mol	NIST Webbook
gf	293.58	kJ/mol	Joback Method
hf	259.00	kJ/mol	NIST Webbook
hfl	231.00 ± 0.80	kJ/mol	NIST Webbook
hfus	9.09	kJ/mol	Joback Method
hvap	27.00 ± 1.00	kJ/mol	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	9.27 ± 0.02	eV	NIST Webbook
ie	9.23 ± 0.01	eV	NIST Webbook
ie	9.30 ± 0.03	eV	NIST Webbook
ie	9.25 ± 0.02	eV	NIST Webbook
log10ws	-1.56		Crippen Method
logp	1.196		Crippen Method
mcvol	68.410	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
rinpol	456.00		NIST Webbook
rinpol	456.00		NIST Webbook

rinpol	457.00		NIST Webbook
rinpol	456.00		NIST Webbook
rinpol	457.00		NIST Webbook
tb	305.30 ± 0.30	K	NIST Webbook
tb	305.20	K	NIST Webbook
tb	305.40 ± 1.50	K	NIST Webbook
tb	307.00 ± 5.00	K	NIST Webbook
tc	482.63	K	Joback Method
tf	177.36	K	Joback Method
vc	0.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	97.07	J/mol×K	300.48	Joback Method
cpg	103.77	J/mol×K	330.84	Joback Method
cpg	110.12	J/mol×K	361.20	Joback Method
cpg	116.15	J/mol×K	391.55	Joback Method
cpg	121.87	J/mol×K	421.91	Joback Method
cpg	127.29	J/mol×K	452.27	Joback Method
cpg	132.43	J/mol×K	482.63	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78808&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions

hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume