1-Buten-3-yne

Other names:	1-BUTEN-3-YEN
	1-Butene-3-yne
	1-Butenyne
	1-Butyn-3-ene
	3-Buten-1-yne
	BUTENYNE
	But-1-en-3-yne
	Buten-3-yne
	ETHYNYLETHENE
	Ethene, ethynyl-
	Monovinylacetylene
	Vinylacetylene
	Vinylethyne
Inchi:	InChI=1S/C4H4/c1-3-4-2/h1,4H,2H2
InchiKey:	WFYPICNXBKQZGB-UHFFFAOYSA-N
Formula:	C4H4
SMILES:	C#CC=C
Mol. weight [g/mol]:	52.07
CAS:	689-97-4

Physical Properties

Property code	Value	Unit	Source
af	0.0920		KDB
chl	-2380.00	kJ/mol	NIST Webbook
gf	306.20	kJ/mol	KDB
hf	295.00	kJ/mol	NIST Webbook
hf	304.80	kJ/mol	KDB
hfus	7.81	kJ/mol	Joback Method
hvap	23.69	kJ/mol	Joback Method
ie	9.90	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.58 ± 0.02	eV	NIST Webbook
ie	9.58 ± 0.02	eV	NIST Webbook
ie	9.58 ± 0.02	eV	NIST Webbook
ie	9.58 ± 0.02	eV	NIST Webbook
ie	9.87	eV	NIST Webbook
ie	9.90	eV	NIST Webbook

ie	9.64 ± 0.03	eV	NIST Webbook
ie	9.63	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
log10ws	-1.15		Crippen Method
logp	0.806		Crippen Method
mcvol	54.320	ml/mol	McGowan Method
pc	4960.00	kPa	KDB
rinpol	373.00		NIST Webbook
rinpol	410.00		NIST Webbook
rinpol	407.15		NIST Webbook
rinpol	374.00		NIST Webbook
rinpol	374.00		NIST Webbook
rinpol	373.00		NIST Webbook
rinpol	404.00		NIST Webbook
tb	278.10	K	KDB
tb	276.15 ± 3.00	K	NIST Webbook
tc	455.00	K	KDB
tf	227.60	K	KDB
vc	0.202	m3/kmol	KDB
zc	0.2648410		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.89	J/mol×K	425.03	Joback Method
cpg	70.14	J/mol×K	277.72	Joback Method
cpg	74.98	J/mol×K	307.18	Joback Method
cpg	79.56	J/mol×K	336.64	Joback Method
cpg	83.89	J/mol×K	366.11	Joback Method
cpg	88.00	J/mol×K	395.57	Joback Method
cpg	95.56	J/mol×K	454.49	Joback Method
hvapt	24.48	kJ/mol	278.10	KDB
hvapt	26.00	kJ/mol	229.00	NIST Webbook
rhol	710.00	kg/m3	273.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35875e+01
Coeff. B	-1.93992e+03
Coeff. C	-5.98620e+01
Temperature range (K), min.	205.72
Temperature range (K), max.	297.13

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.14672e+01
Coeff. B	-5.12322e+03
Coeff. C	-8.71388e+00
Coeff. D	7.76544e-06
Temperature range (K), min.	179.95
Temperature range (K), max.	454.00

Sources

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=401
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/mol401.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C689974&Units=SI

Legend

af:	Acentric Factor
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

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
pvap:	Vapor 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
vc:	Critical Volume
zc:	Critical Compressibility