3-Penten-1-yne, (E)-

Other names:	(E)-3-Penten-1-yne
	(E)-CH3CH=CHC«equiv»CH
	(E)-CH3CH=CHCÂ«equivÂ»CH
	3-Pentene-1-yne, (E)-
	Pent-1-yn-3-ene, (E)-
	trans-2-Penten-4-Yne
	trans-3-Penten-1-Yne
Inchi:	InChI=1S/C5H6/c1-3-5-4-2/h1,4-5H,2H3/b5-4+
InchiKey:	XAJOPMVSQIBJCW-SNAWJCMRSA-N
Formula:	C5H6
SMILES:	C#CC=CC
Mol. weight [g/mol]:	66.10
CAS:	2004-69-5

Physical Properties

Property code	Value	Unit	Source
gf	294.51	kJ/mol	Joback Method
hf	259.00	kJ/mol	NIST Webbook
hfus	11.88	kJ/mol	Joback Method
hvap	26.54	kJ/mol	Joback Method
ie	9.05 ± 0.01	eV	NIST Webbook
ie	9.10 ± 0.10	eV	NIST Webbook
ie	9.11 ± 0.03	eV	NIST Webbook
log10ws	-1.56		Crippen Method
logp	1.196		Crippen Method
mcvol	68.410	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	325.05 ± 0.40	K	NIST Webbook
tb	323.65 ± 1.00	K	NIST Webbook
tc	492.89	K	Joback Method
tf	188.00	K	Joback Method
vc	0.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	94.90	J/mol×K	308.08	Joback Method
cpg	101.94	J/mol×K	338.88	Joback Method
cpg	108.58	J/mol×K	369.68	Joback Method
cpg	114.84	J/mol×K	400.48	Joback Method
cpg	120.73	J/mol×K	431.29	Joback Method
cpg	126.28	J/mol×K	462.09	Joback Method
cpg	131.51	J/mol×K	492.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54585e+01
Coeff. B	-3.16592e+03
Coeff. C	-3.15970e+01
Temperature range (K), min.	240.28
Temperature range (K), max.	343.60

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=C2004695&Units=SI

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

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

Legend

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume