1-Penten-3-yne

Other names:	1-Pentene-3-yne
	CH2=CHC«equiv»CCH3
	CH2=CHCÂ«equivÂ»CCH3
	Methyl vinylacetylene
	Pyrylen
	Pyrylene
	Vinylmethylacetylene
Inchi:	InChI=1S/C5H6/c1-3-5-4-2/h3H,1H2,2H3
InchiKey:	FILUFGAZMJGNEN-UHFFFAOYSA-N
Formula:	C5H6
SMILES:	C=CC#CC
Mol. weight [g/mol]:	66.10
CAS:	646-05-9

Physical Properties

Property code	Value	Unit	Source
gf	281.86	kJ/mol	Joback Method
hf	251.20	kJ/mol	Joback Method
hfus	10.55	kJ/mol	Joback Method
hvap	28.21	kJ/mol	Joback Method
ie	9.06 ± 0.03	eV	NIST Webbook
ie	9.00 ± 0.01	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	9.10 ± 0.10	eV	NIST Webbook
ie	9.00 ± 0.01	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
log10ws	-1.56		Crippen Method
logp	1.196		Crippen Method
mcvol	68.410	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
tb	332.40 ± 1.00	K	NIST Webbook
tb	332.40 ± 3.00	K	NIST Webbook
tb	332.70	K	NIST Webbook
tc	512.78	K	Joback Method
tf	250.45	K	Joback Method
vc	0.259	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	94.83	J/mol×K	319.48	Joback Method
cpg	101.40	J/mol×K	351.70	Joback Method
cpg	107.70	J/mol×K	383.91	Joback Method
cpg	113.73	J/mol×K	416.13	Joback Method
cpg	119.51	J/mol×K	448.35	Joback Method
cpg	125.04	J/mol×K	480.57	Joback Method
cpg	130.34	J/mol×K	512.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43681e+01
Coeff. B	-2.91825e+03
Coeff. C	-3.33850e+01
Temperature range (K), min.	240.64
Temperature range (K), max.	355.61

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C646059&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

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

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