1,3-Hexadien-5-yne

Other names:	Butadienylacetylene
	HC«equiv»CCH=CHCH=CH2
	HCÂ«equivÂ»CCH=CHCH=CH2
Inchi:	InChI=1S/C6H6/c1-3-5-6-4-2/h1,4-6H,2H2
InchiKey:	OGWJYLKDZYZYBA-UHFFFAOYSA-N
Formula:	C6H6
SMILES:	C#CC=CC=C
Mol. weight [g/mol]:	78.11
CAS:	10420-90-3

Physical Properties

Property code	Value	Unit	Source
gf	390.77	kJ/mol	Joback Method
hf	367.38	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	28.10	kJ/mol	Joback Method
ie	9.20	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	1.362		Crippen Method
mcvol	78.200	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	670.00		NIST Webbook
tb	358.00 ± 2.00	K	NIST Webbook
tc	516.95	K	Joback Method
tf	197.51	K	Joback Method
vc	0.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.90	J/mol×K	485.40	Joback Method
cpg	112.82	J/mol×K	327.64	Joback Method
cpg	120.78	J/mol×K	359.19	Joback Method

cpg	128.24	J/mol×K	390.74	Joback Method
cpg	135.23	J/mol×K	422.30	Joback Method
cpg	141.78	J/mol×K	453.85	Joback Method
cpg	153.64	J/mol×K	516.95	Joback Method
hvapt	44.00	kJ/mol	263.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31124e+01
Coeff. B	-2.47150e+03
Coeff. C	-6.70330e+01
Temperature range (K), min.	233.00
Temperature range (K), max.	383.85

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=C10420903&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume