1,5-Hexadien-3-yne

Other names:	1,5-Hexadiene-3-yne
	CH2=CHC«equiv»CCH=CH2
	CH2=CHCÂ«equivÂ»CCH=CH2
	Divinylacetylene
Inchi:	InChI=1S/C6H6/c1-3-5-6-4-2/h3-4H,1-2H2
InchiKey:	AUBDSFLQOBEOPX-UHFFFAOYSA-N
Formula:	C6H6
SMILES:	C=CC#CC=C
Mol. weight [g/mol]:	78.11
CAS:	821-08-9

Physical Properties

Property code	Value	Unit	Source
gf	378.12	kJ/mol	Joback Method
hf	355.99	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	29.76	kJ/mol	Joback Method
ie	8.50 ± 0.02	eV	NIST Webbook
ie	8.50 ± 0.02	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	1.362		Crippen Method
mcvol	78.200	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	679.00		NIST Webbook
rinpol	679.00		NIST Webbook
tb	357.90 ± 1.50	K	NIST Webbook
tc	536.61	K	Joback Method
tf	259.96	K	Joback Method
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	146.86	J/mol×K	503.68	Joback Method
cpg	112.63	J/mol×K	339.04	Joback Method
cpg	120.20	J/mol×K	371.97	Joback Method
cpg	127.39	J/mol×K	404.90	Joback Method
cpg	134.22	J/mol×K	437.82	Joback Method
cpg	140.71	J/mol×K	470.75	Joback Method
cpg	152.71	J/mol×K	536.61	Joback Method
hvapt	40.40	kJ/mol	290.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	8.17183e+00
Coeff. B	-7.50409e+02
Coeff. C	-1.48526e+02
Temperature range (K), min.	223.00
Temperature range (K), max.	410.87

Sources

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=C821089&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

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