1,3-Hexadiyne

Inchi: InChI=1S/C6H6/c1-3-5-6-4-2/h1H,4H2,2H3
InchiKey: AKOJBFZCIRFXBA-UHFFFAOYSA-N
Formula: C6H6
SMILES: C#CC#CCC
Mol. weight [g/mol]: 78.11
CAS: 4447-21-6

Physical Properties

Property code	Value	Unit	Source
gf	425.51	kJ/mol	Joback Method
hf	397.03	kJ/mol	Joback Method
hfus	17.39	kJ/mol	Joback Method
hvap	30.96	kJ/mol	Joback Method
ie	9.41	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
log10ws	-1.92		Crippen Method
logp	1.033		Crippen Method
mcvol	78.200	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
rinpol	688.00		NIST Webbook
tb	335.80	K	Joback Method
tc	539.44	K	Joback Method
tf	310.45	K	Joback Method
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.53	J/mol×K	335.80	Joback Method
cpg	125.52	J/mol×K	369.74	Joback Method
cpg	132.19	J/mol×K	403.68	Joback Method
cpg	138.54	J/mol×K	437.62	Joback Method
cpg	144.58	J/mol×K	471.56	Joback Method
cpg	150.34	J/mol×K	505.50	Joback Method

cpg	155.83	J/mol×K	539.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.20	K	26.70	NIST Webbook
tbrp	300.20	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63560e+01
Coeff. B	-3.77529e+03
Coeff. C	-4.23740e+01
Temperature range (K), min.	277.33
Temperature range (K), max.	384.20

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4447216&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume