1,5-Hexadiyne

Other names:	Bipropargyl
	Dipropargyl
	HCCCH2CH2CCH
	hexa-1,5-diyne
Inchi:	InChI=1S/C6H6/c1-3-5-6-4-2/h1-2H,5-6H2
InchiKey:	YFIBSNDOVCWPBL-UHFFFAOYSA-N
Formula:	C6H6
SMILES:	C#CCCC#C
Mol. weight [g/mol]:	78.11
CAS:	628-16-0

Physical Properties

Property code	Value	Unit	Source
gf	445.78	kJ/mol	Joback Method
hf	416.63	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	28.67	kJ/mol	Joback Method
ie	10.48	eV	NIST Webbook
ie	9.93 ± 0.05	eV	NIST Webbook
ie	9.98 ± 0.05	eV	NIST Webbook
ie	9.90 ± 0.02	eV	NIST Webbook
ie	9.87 ± 0.03	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	10.35	eV	NIST Webbook
log10ws	-1.92		Crippen Method
logp	1.033		Crippen Method
mcvol	78.200	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
rinpol	680.00		NIST Webbook
rinpol	680.00		NIST Webbook
tb	359.15 ± 1.50	K	NIST Webbook
tb	361.00 ± 0.15	K	NIST Webbook
tb	358.60 ± 3.00	K	NIST Webbook
tb	360.00 ± 6.00	K	NIST Webbook
tb	359.00	K	NIST Webbook
tc	505.20	K	Joback Method
tf	267.00 ± 4.00	K	NIST Webbook

vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.84	J/mol×K	316.92	Joback Method
cpg	127.81	J/mol×K	348.30	Joback Method
cpg	134.41	J/mol×K	379.68	Joback Method
cpg	140.64	J/mol×K	411.06	Joback Method
cpg	146.53	J/mol×K	442.44	Joback Method
cpg	152.09	J/mol×K	473.82	Joback Method
cpg	157.35	J/mol×K	505.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34210e+01
Coeff. B	-2.60510e+03
Coeff. C	-6.30560e+01
Temperature range (K), min.	261.41
Temperature range (K), max.	384.30

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C628160&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

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