2,4-Hexadiyne

Other names:	CH3C«equiv»CC«equiv»CCH3
	CH3CÂ«equivÂ»CCÂ«equivÂ»CCH3
	Dimethylbutadiyne
	Dimethyldiacetylene
	Hexa-2,4-diyne
Inchi:	InChI=1S/C6H6/c1-3-5-6-4-2/h1-2H3
InchiKey:	PCTCNWZFDASPLA-UHFFFAOYSA-N
Formula:	C6H6
SMILES:	CC#CC#CC
Mol. weight [g/mol]:	78.11
CAS:	2809-69-0

Physical Properties

Property code	Value	Unit	Source
chl	-3553.70 ± 4.90	kJ/mol	NIST Webbook
gf	405.24	kJ/mol	Joback Method
hf	377.40	kJ/mol	NIST Webbook
hfl	335.20 ± 5.00	kJ/mol	NIST Webbook
hfus	17.54	kJ/mol	Joback Method
hvap	42.50	kJ/mol	NIST Webbook
hvap	42.20	kJ/mol	NIST Webbook
ie	8.90 ± 0.05	eV	NIST Webbook
ie	9.08	eV	NIST Webbook
ie	8.92 ± 0.02	eV	NIST Webbook
ie	11.51 ± 0.02	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	8.91	eV	NIST Webbook
ie	9.00 ± 0.10	eV	NIST Webbook
ie	8.92	eV	NIST Webbook
log10ws	-1.92		Crippen Method
logp	1.033		Crippen Method
mcvol	78.200	ml/mol	McGowan Method
pc	4602.62	kPa	Joback Method
rinpol	891.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	891.00		NIST Webbook
ss	178.14	J/mol×K	NIST Webbook

tb	402.50 ± 0.50	K	NIST Webbook
tb	403.00 ± 3.00	K	NIST Webbook
tb	402.70	K	NIST Webbook
tc	574.27	K	Joback Method
tf	338.00 ± 3.00	K	NIST Webbook
tf	337.00 ± 2.00	K	NIST Webbook
tt	337.84 ± 0.15	K	NIST Webbook
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.54	J/mol×K	501.07	Joback Method
cpg	148.62	J/mol×K	537.67	Joback Method
cpg	115.74	J/mol×K	354.68	Joback Method
cpg	122.83	J/mol×K	391.28	Joback Method
cpg	129.65	J/mol×K	427.88	Joback Method
cpg	136.22	J/mol×K	464.47	Joback Method
cpg	154.46	J/mol×K	574.27	Joback Method
cps	133.57	J/mol×K	298.15	NIST Webbook
hfust	1.00	kJ/mol	117.90	NIST Webbook
hsubt	47.00 ± 2.00	kJ/mol	307.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63307e+01
Coeff. B	-4.09247e+03
Coeff. C	-5.30870e+01
Temperature range (K), min.	308.18
Temperature range (K), max.	424.48

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2809690&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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