

# 2,4-Hexadiyne

<b>Other names:</b>	CH <sub>3</sub> C«equiv»CC«equiv»CCH <sub>3</sub> CH <sub>3</sub> CÂ«equivÂ»CCÂ«equivÂ»CCH <sub>3</sub> Dimethylbutadiyne Dimethyldiacetylene Hexa-2,4-diyne
<b>Inchi:</b>	InChI=1S/C6H6/c1-3-5-6-4-2/h1-2H3
<b>InchiKey:</b>	PCTCNWZFDASPLA-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>6</sub> H <sub>6</sub>
<b>SMILES:</b>	CC#CC#CC
<b>Mol. weight [g/mol]:</b>	78.11
<b>CAS:</b>	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	8.92	eV	NIST Webbook
ie	9.00 ± 0.10	eV	NIST Webbook
ie	8.91	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	11.51 ± 0.02	eV	NIST Webbook
ie	9.08	eV	NIST Webbook
ie	8.92 ± 0.02	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/molxK	NIST Webbook

tb	402.70	K	NIST Webbook
tb	403.00 ± 3.00	K	NIST Webbook
tb	402.50 ± 0.50	K	NIST Webbook
tc	574.27	K	Joback Method
tf	337.00 ± 2.00	K	NIST Webbook
tf	338.00 ± 3.00	K	NIST Webbook
tt	337.84 ± 0.15	K	NIST Webbook
vc	0.295	m <sup>3</sup> /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	$\ln(P_{vp}) = A + B/(T + C)$
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

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2809690&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2809690&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>p vap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ss:</b>	Solid phase molar entropy at standard conditions
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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