

1-Hexen-3-yne, 2-methyl-

Other names:	2-Methyl-1-hexen-3-yne C2H5C«equiv»CC(CH3)=CH2 C2H5CÂ«equivÂ»CC(CH3)=CH2
Inchi:	InChI=1S/C7H10/c1-4-5-6-7(2)3/h2,4H2,1,3H3
InchiKey:	IXPWKHNDQICVPZ-UHFFFAOYSA-N
Formula:	C7H10
SMILES:	C=C(C)C#CCC
Mol. weight [g/mol]:	94.15
CAS:	23056-94-2

Physical Properties

Property code	Value	Unit	Source
gf	290.15	kJ/mol	Joback Method
hf	200.13	kJ/mol	Joback Method
hfus	14.42	kJ/mol	Joback Method
hvap	32.74	kJ/mol	Joback Method
ie	8.66 ± 0.01	eV	NIST Webbook
log10ws	-2.40		Crippen Method
logp	1.976		Crippen Method
mcvol	96.590	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	377.60	K	NIST Webbook
tc	561.71	K	Joback Method
tf	259.03	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.33	J/mol×K	365.12	Joback Method
cpg	168.43	J/mol×K	397.88	Joback Method
cpg	178.09	J/mol×K	430.65	Joback Method
cpg	187.32	J/mol×K	463.41	Joback Method
cpg	196.14	J/mol×K	496.18	Joback Method

cpg	204.56	J/mol×K	528.94	Joback Method
cpg	212.60	J/mol×K	561.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.68343e+01
Coeff. B	-4.00840e+03
Coeff. C	-4.94730e+01
Temperature range (K), min.	291.72
Temperature range (K), max.	397.34

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23056942&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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