2-Hexyne, 5-methyl-

Other names:	1-Methyl-2-isobutylacetylene
	5-Methyl-2-hexyne
	METHYLISOBUTYLACETYLENE
	Methyl isobutylacetylene
Inchi:	InChI=1S/C7H12/c1-4-5-6-7(2)3/h7H,6H2,1-3H3
InchiKey:	SVGAHRUSRQTQES-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CC#CCC(C)C
Mol. weight [g/mol]:	96.17
CAS:	53566-37-3

Physical Properties

Property code	Value	Unit	Source
gf	208.42	kJ/mol	Joback Method
hf	79.21	kJ/mol	Joback Method
hfus	13.48	kJ/mol	Joback Method
hvap	32.94	kJ/mol	Joback Method
ie	9.32 ± 0.01	eV	NIST Webbook
log10ws	-2.31		Crippen Method
logp	2.056		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	701.00		NIST Webbook
rinpol	701.00		NIST Webbook
tb	375.61 ± 0.30	K	NIST Webbook
tb	375.29 ± 0.30	K	NIST Webbook
tb	376.00 ± 6.00	K	NIST Webbook
tb	375.00	K	NIST Webbook
tc	561.09	K	Joback Method
tf	259.75	K	Joback Method
tt	180.54 ± 0.20	K	NIST Webbook
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.85	J/mol×K	368.12	Joback Method
cpg	182.83	J/mol×K	400.28	Joback Method
cpg	193.38	J/mol×K	432.44	Joback Method
cpg	203.51	J/mol×K	464.60	Joback Method
cpg	213.23	J/mol×K	496.76	Joback Method
cpg	222.56	J/mol×K	528.92	Joback Method
cpg	231.49	J/mol×K	561.09	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37983e+01
Coeff. B	-2.92657e+03
Coeff. C	-5.68120e+01
Temperature range (K), min.	273.42
Temperature range (K), max.	401.65

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol421.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53566373&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume