1-Pentyne, 4-methyl-

Other names: (CH3)2CHCH2C«equiv»CH
(CH3)2CHCH2CÂ«equivÂ»CH
4-METHYL-1-PENTYNE
ISOBUTYLACETYLENE
ISOBUTYLETHYNE
Inchi: InChI=1S/C6H10/c1-4-5-6(2)3/h1,6H,5H2,2-3H3
InchiKey: OXRWICUICBZVAE-UHFFFAOYSA-N
Formula: C6H10
SMILES: C#CCC(C)C
Mol. weight [g/mol]: 82.14
CAS: 7154-75-8

Physical Properties

Property code	Value	Unit	Source
gf	220.27	kJ/mol	Joback Method
hf	119.45	kJ/mol	Joback Method
hfus	10.75	kJ/mol	Joback Method
hvap	28.42	kJ/mol	Joback Method
ie	9.83 ± 0.05	eV	NIST Webbook
ie	10.05 ± 0.01	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.666		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
rinpol	550.00		NIST Webbook
rinpol	553.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	553.00		NIST Webbook
rinpol	552.00		NIST Webbook
tb	334.40	K	NIST Webbook
tb	334.45 ± 0.50	K	NIST Webbook
tb	334.30 ± 0.50	K	NIST Webbook
tb	334.90 ± 2.00	K	NIST Webbook
tb	334.32 ± 0.30	K	NIST Webbook
tc	505.86	K	Joback Method
tf	167.85 ± 0.40	K	NIST Webbook
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.67	J/mol×K	326.36	Joback Method
cpg	147.86	J/mol×K	356.28	Joback Method
cpg	156.66	J/mol×K	386.19	Joback Method
cpg	165.08	J/mol×K	416.11	Joback Method
cpg	173.13	J/mol×K	446.03	Joback Method
cpg	180.83	J/mol×K	475.94	Joback Method
cpg	188.19	J/mol×K	505.86	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37819e+01
Coeff. B	-2.60607e+03
Coeff. C	-5.02550e+01
Temperature range (K), min.	243.38
Temperature range (K), max.	357.92

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol411.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7154758&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