4-Methyl-2-pentyne

Other names: 2-Pentyne, 4-methyl-
Inchi: InChI=1S/C6H10/c1-4-5-6(2)3/h6H,1-3H3
InchiKey: SLMFWJQZLPEDDU-UHFFFAOYSA-N
Formula: C6H10
SMILES: CC#CC(C)C
Mol. weight [g/mol]: 82.14
CAS: 21020-27-9

Physical Properties

Property code	Value	Unit	Source
gf	200.00	kJ/mol	Joback Method
hf	99.85	kJ/mol	Joback Method
hfus	10.89	kJ/mol	Joback Method
hvap	30.71	kJ/mol	Joback Method
ie	9.31 ± 0.05	eV	NIST Webbook
ie	9.35 ± 0.01	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.666		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	615.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	594.00		NIST Webbook
tb	345.40 ± 1.00	K	NIST Webbook
tb	346.00	K	NIST Webbook
tb	345.90 ± 0.30	K	NIST Webbook
tb	346.28 ± 0.30	K	NIST Webbook
tb	346.15 ± 0.40	K	NIST Webbook
tc	538.95	K	Joback Method
tf	162.78 ± 0.30	K	NIST Webbook
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.87	J/mol×K	345.24	Joback Method
cpg	147.26	J/mol×K	377.53	Joback Method
cpg	156.29	J/mol×K	409.81	Joback Method
cpg	164.98	J/mol×K	442.10	Joback Method
cpg	173.32	J/mol×K	474.38	Joback Method
cpg	181.34	J/mol×K	506.67	Joback Method
cpg	189.03	J/mol×K	538.95	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37418e+01
Coeff. B	-2.66783e+03
Coeff. C	-5.27350e+01
Temperature range (K), min.	251.02
Temperature range (K), max.	369.19

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol412.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21020279&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