1-Hexyne, 5-methyl-

Other names: (CH3)2CH(CH2)2C«equiv»CH
(CH3)2CH(CH2)2CÂ«equivÂ»CH
5-Methyl-1-hexyne
Inchi: InChI=1S/C7H12/c1-4-5-6-7(2)3/h1,7H,5-6H2,2-3H3
InchiKey: HKNANEMUCJGPMS-UHFFFAOYSA-N
Formula: C7H12
SMILES: C#CCCC(C)C
Mol. weight [g/mol]: 96.17
CAS: 2203-80-7

Physical Properties

Property code	Value	Unit	Source
gf	228.69	kJ/mol	Joback Method
hf	98.81	kJ/mol	Joback Method
hfus	13.34	kJ/mol	Joback Method
hvap	30.65	kJ/mol	Joback Method
ie	10.02 ± 0.01	eV	NIST Webbook
log10ws	-2.31		Crippen Method
logp	2.056		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	656.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	654.00		NIST Webbook
tb	364.65 ± 1.50	K	NIST Webbook
tb	363.95 ± 0.70	K	NIST Webbook
tb	365.00 ± 0.20	K	NIST Webbook
tb	365.15 ± 2.00	K	NIST Webbook
tb	364.90	K	NIST Webbook
tb	365.20	K	NIST Webbook
tc	528.78	K	Joback Method
tf	148.55 ± 0.50	K	NIST Webbook
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.87	J/mol×K	349.24	Joback Method
cpg	182.56	J/mol×K	379.16	Joback Method
cpg	192.80	J/mol×K	409.09	Joback Method
cpg	202.59	J/mol×K	439.01	Joback Method
cpg	211.96	J/mol×K	468.93	Joback Method
cpg	220.92	J/mol×K	498.86	Joback Method
cpg	229.49	J/mol×K	528.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38742e+01
Coeff. B	-2.86792e+03
Coeff. C	-5.51500e+01
Temperature range (K), min.	266.23
Temperature range (K), max.	390.08

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/mol419.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2203807&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
vc:	Critical Volume