1-Hexene, 5-methyl-

Other names: 5-Methyl-1-hexene
5-methylhex-1-ene
Inchi: InChI=1S/C7H14/c1-4-5-6-7(2)3/h4,7H,1,5-6H2,2-3H3
InchiKey: JIUFYGIESXPUPL-UHFFFAOYSA-N
Formula: C7H14
SMILES: C=CCCC(C)C
Mol. weight [g/mol]: 98.19
CAS: 3524-73-0

Physical Properties

Property code	Value	Unit	Source
chl	-4655.37 ± 0.50	kJ/mol	NIST Webbook
gf	93.46	kJ/mol	Joback Method
hf	-67.66	kJ/mol	Joback Method
hfus	9.08	kJ/mol	Joback Method
hvap	34.30	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	655.50		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	639.40		NIST Webbook
rinpol	658.20		NIST Webbook
rinpol	650.60		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	649.30		NIST Webbook

rinpol	650.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	653.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	649.30		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	656.40		NIST Webbook
rinpol	655.50		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	649.00		NIST Webbook
tb	355.80	K	Joback Method
tc	528.70	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	151.89	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.32	J/mol×K	355.80	Joback Method
cpg	191.94	J/mol×K	384.29	Joback Method
cpg	203.10	J/mol×K	412.77	Joback Method
cpg	213.82	J/mol×K	441.26	Joback Method
cpg	224.10	J/mol×K	469.74	Joback Method
cpg	233.97	J/mol×K	498.23	Joback Method
cpg	243.44	J/mol×K	526.72	Joback Method
dvisc	0.0078928	Pa×s	151.89	Joback Method
dvisc	0.0025390	Pa×s	185.88	Joback Method
dvisc	0.0011597	Pa×s	219.86	Joback Method
dvisc	0.0006534	Pa×s	253.84	Joback Method
dvisc	0.0004215	Pa×s	287.83	Joback Method
dvisc	0.0002983	Pa×s	321.82	Joback Method
dvisc	0.0002256	Pa×s	355.80	Joback Method

hvapt	33.50	kJ/mol	353.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40537e+01
Coeff. B	-2.92081e+03
Coeff. C	-4.88990e+01
Temperature range (K), min.	261.07
Temperature range (K), max.	383.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol221.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3524730&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
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