1-Hexene, 5,5-dimethyl-

Other names: 5,5-Dimethyl-1-hexene
5,5-Dimethylhex-1-ene
5,5-Dimethylhexene-1
Inchi: InChI=1S/C8H16/c1-5-6-7-8(2,3)4/h5H,1,6-7H2,2-4H3
InchiKey: KZJIOVQKSAOPOP-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=CCCC(C)(C)C
Mol. weight [g/mol]: 112.21
CAS: 7116-86-1

Physical Properties

Property code	Value	Unit	Source
gf	107.16	kJ/mol	Joback Method
hf	-91.77	kJ/mol	Joback Method
hfus	7.78	kJ/mol	Joback Method
hvap	37.70	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	711.50		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	704.40		NIST Webbook
rinpol	711.50		NIST Webbook
tb	374.00 ± 4.00	K	NIST Webbook
tb	376.30 ± 0.50	K	NIST Webbook
tc	553.76	K	Joback Method
tf	180.58	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.61	J/mol×K	375.89	Joback Method

cpg	232.71	J/mol×K	405.54	Joback Method
cpg	246.11	J/mol×K	435.18	Joback Method
cpg	258.84	J/mol×K	464.83	Joback Method
cpg	270.93	J/mol×K	494.47	Joback Method
cpg	282.41	J/mol×K	524.12	Joback Method
cpg	293.30	J/mol×K	553.76	Joback Method
dvisc	0.0095731	Pa×s	180.58	Joback Method
dvisc	0.0033567	Pa×s	213.13	Joback Method
dvisc	0.0015537	Pa×s	245.68	Joback Method
dvisc	0.0008612	Pa×s	278.24	Joback Method
dvisc	0.0005402	Pa×s	310.79	Joback Method
dvisc	0.0003702	Pa×s	343.34	Joback Method
dvisc	0.0002708	Pa×s	375.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.22862e+01
Coeff. B	-2.51659e+03
Coeff. C	-6.51540e+01
Temperature range (K), min.	274.89
Temperature range (K), max.	425.97

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/mol291.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7116861&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
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
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