1-Hexene, 4,5-dimethyl-

Other names: 4,5-Dimethyl-1-hexene
4,5-Dimethylhex-1-ene
Inchi: InChI=1S/C8H16/c1-5-6-8(4)7(2)3/h5,7-8H,1,6H2,2-4H3
InchiKey: UFWIBUBEFUNVNI-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=CCC(C)C(C)C
Mol. weight [g/mol]: 112.21
CAS: 16106-59-5

Physical Properties

Property code	Value	Unit	Source
gf	99.44	kJ/mol	Joback Method
hf	-93.58	kJ/mol	Joback Method
hfus	8.15	kJ/mol	Joback Method
hvap	38.50	kJ/mol	NIST Webbook
log10ws	-2.54		Crippen Method
logp	2.855		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	735.00		NIST Webbook
rinpol	131.20		NIST Webbook
rinpol	747.40		NIST Webbook
rinpol	740.80		NIST Webbook
rinpol	131.20		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	747.40		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	742.00		NIST Webbook
tb	378.24	K	Joback Method
tc	552.91	K	Joback Method
tf	148.16	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.47	J/mol×K	378.24	Joback Method
cpg	278.59	J/mol×K	523.80	Joback Method
cpg	267.38	J/mol×K	494.69	Joback Method
cpg	255.68	J/mol×K	465.57	Joback Method
cpg	243.47	J/mol×K	436.46	Joback Method
cpg	230.74	J/mol×K	407.35	Joback Method
cpg	289.32	J/mol×K	552.91	Joback Method
dvisc	0.0002238	Pa×s	378.24	Joback Method
dvisc	0.0003084	Pa×s	339.89	Joback Method
dvisc	0.0004609	Pa×s	301.55	Joback Method
dvisc	0.0007745	Pa×s	263.20	Joback Method
dvisc	0.0015535	Pa×s	224.85	Joback Method
dvisc	0.0041486	Pa×s	186.51	Joback Method
dvisc	0.0184203	Pa×s	148.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30165e+01
Coeff. B	-2.82045e+03
Coeff. C	-5.75110e+01
Temperature range (K), min.	279.09
Temperature range (K), max.	423.57

Sources

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=290

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16106595&Units=SI

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