3-Hexene, 2,5-dimethyl-, (E)-

Other names:	(3E)-2,5-Dimethyl-3-hexene
	(E)-(CH3)2CHCH=CHCH(CH3)2
	(E)-2,5-DIMETHYL-3-HEXENE
	(E)-2,5-Dimethylhex-3-ene
	2,5-DIMETHYL-TRANS-3-HEXENE
	TRANS-2,5-DIMETHYL-3-HEXENE
	trans-Diisopropylethylene
Inchi:	InChI=1S/C8H16/c1-7(2)5-6-8(3)4/h5-8H,1-4H3/b6-5+
InchiKey:	KNCMKWVOMRUHKZ-AATRIKPKSA-N
Formula:	C8H16
SMILES:	CC(C)C=CC(C)C
Mol. weight [g/mol]:	112.21
CAS:	692-70-6

Physical Properties

Property code	Value	Unit	Source
chl	-5275.50 ± 1.50	kJ/mol	NIST Webbook
chl	-5265.56 ± 0.50	kJ/mol	NIST Webbook
gf	91.82	kJ/mol	Joback Method
hf	-119.50	kJ/mol	NIST Webbook
hfl	-159.30 ± 1.50	kJ/mol	NIST Webbook
hfus	9.63	kJ/mol	Joback Method
hvap	37.50	kJ/mol	NIST Webbook
ie	8.84 ± 0.01	eV	NIST Webbook
log10ws	-2.54		Crippen Method
logp	2.855		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	704.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	703.20		NIST Webbook
rinpol	703.70		NIST Webbook
rinpol	713.60		NIST Webbook
rinpol	695.00		NIST Webbook

rinpol	695.00		NIST Webbook
rinpol	695.50		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	694.50		NIST Webbook
tb	375.19 ± 0.20	K	NIST Webbook
tb	375.24 ± 0.30	K	NIST Webbook
tc	565.78	K	Joback Method
tf	177.93 ± 0.03	K	NIST Webbook
tf	177.95 ± 0.02	K	NIST Webbook
tf	177.92 ± 0.04	K	NIST Webbook
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.83	J/mol×K	385.72	Joback Method
cpg	280.44	J/mol×K	535.77	Joback Method
cpg	269.06	J/mol×K	505.76	Joback Method
cpg	257.12	J/mol×K	475.75	Joback Method
cpg	244.62	J/mol×K	445.74	Joback Method
cpg	231.54	J/mol×K	415.73	Joback Method
cpg	291.30	J/mol×K	565.78	Joback Method
dvisc	0.0001887	Pa×s	385.72	Joback Method
dvisc	0.0002641	Pa×s	345.57	Joback Method
dvisc	0.0004036	Pa×s	305.43	Joback Method
dvisc	0.0007016	Pa×s	265.28	Joback Method
dvisc	0.0014851	Pa×s	225.13	Joback Method
dvisc	0.0043531	Pa×s	184.99	Joback Method
dvisc	0.0231611	Pa×s	144.84	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37940e+01
Coeff. B	-2.87756e+03

Coeff. C	-6.15820e+01
Temperature range (K), min.	274.63
Temperature range (K), max.	400.82

Sources

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=317
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C692706&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
hfl:	Liquid phase 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