2-Hexene, 2,3-dimethyl-

Other names:	2,3-Dimethyl-2-hexene
	2,3-Dimethylhex-2-ene
	C2H5CH2C(CH3)=C(CH3)2
Inchi:	InChI=1S/C8H16/c1-5-6-8(4)7(2)3/h5-6H2,1-4H3
InchiKey:	RGYAVZGBAJFMIZ-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CCCC(C)=C(C)C
Mol. weight [g/mol]:	112.21
CAS:	7145-20-2

Physical Properties

Property code	Value	Unit	Source
gf	79.60	kJ/mol	Joback Method
hf	-110.81	kJ/mol	Joback Method
hfus	14.06	kJ/mol	Joback Method
hvap	39.70	kJ/mol	NIST Webbook
ie	8.19 ± 0.01	eV	NIST Webbook
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	795.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	787.40		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	788.50		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	789.00		NIST Webbook

rinpol	796.20		NIST Webbook
rinpol	795.20		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	800.20		NIST Webbook
rinpol	787.50		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	797.00		NIST Webbook
tb	395.00 ± 0.40	K	NIST Webbook
tb	394.92 ± 0.40	K	NIST Webbook
tb	395.01 ± 0.30	K	NIST Webbook
tb	395.01 ± 0.07	K	NIST Webbook
tb	395.00 ± 0.40	K	NIST Webbook
tc	565.14	K	Joback Method
tf	158.15 ± 0.03	K	NIST Webbook
tf	158.08 ± 0.06	K	NIST Webbook
tf	158.09 ± 0.04	K	NIST Webbook
tf	155.00 ± 0.80	K	NIST Webbook
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.01	J/mol×K	386.36	Joback Method
cpg	231.36	J/mol×K	416.16	Joback Method
cpg	244.11	J/mol×K	445.95	Joback Method
cpg	256.30	J/mol×K	475.75	Joback Method
cpg	267.94	J/mol×K	505.55	Joback Method
cpg	279.06	J/mol×K	535.34	Joback Method
cpg	289.68	J/mol×K	565.14	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39754e+01
Coeff. B	-3.16840e+03
Coeff. C	-5.64000e+01

Temperature range (K), min.	287.88
Temperature range (K), max.	422.10

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol296.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7145202&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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