3-Heptene, 2-methyl-, (E)-

Other names:	(E)-2-METHYL-3-HEPTENE
	(E)-2-Methylhept-3-ene
	2-METHYL-TRANS-3-HEPTENE
	TRANS-2-METHYL-3-HEPTENE
Inchi:	InChI=1S/C8H16/c1-4-5-6-7-8(2)3/h6-8H,4-5H2,1-3H3/b7-6+
InchiKey:	CYEZJYAMLNTSKN-VOTSOKGWSA-N
Formula:	C8H16
SMILES:	CCCC=CC(C)C
Mol. weight [g/mol]:	112.21
CAS:	692-96-6

Physical Properties

Property code	Value	Unit	Source
gf	94.26	kJ/mol	Joback Method
hf	-96.51	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	38.90	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
rinpol	741.00		NIST Webbook
rinpol	741.10		NIST Webbook
rinpol	751.40		NIST Webbook
rinpol	741.10		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	742.50		NIST Webbook
rinpol	749.40		NIST Webbook
rinpol	750.70		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	754.80		NIST Webbook

rinpol	751.10		NIST Webbook
rinpol	749.40		NIST Webbook
tb	387.13 ± 0.30	K	NIST Webbook
tc	562.05	K	Joback Method
tf	165.63 ± 0.02	K	NIST Webbook
tf	165.59 ± 0.03	K	NIST Webbook
tf	165.59 ± 0.04	K	NIST Webbook
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.94	J/mol×K	386.16	Joback Method
cpg	231.23	J/mol×K	415.47	Joback Method
cpg	243.94	J/mol×K	444.79	Joback Method
cpg	256.10	J/mol×K	474.10	Joback Method
cpg	267.72	J/mol×K	503.42	Joback Method
cpg	278.83	J/mol×K	532.73	Joback Method
cpg	289.43	J/mol×K	562.05	Joback Method
dvisc	0.0101457	Pa×s	159.84	Joback Method
dvisc	0.0028001	Pa×s	197.56	Joback Method
dvisc	0.0011677	Pa×s	235.28	Joback Method
dvisc	0.0006201	Pa×s	273.00	Joback Method
dvisc	0.0003840	Pa×s	310.72	Joback Method
dvisc	0.0002638	Pa×s	348.44	Joback Method
dvisc	0.0001950	Pa×s	386.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38974e+01
Coeff. B	-3.08184e+03
Coeff. C	-5.50000e+01
Temperature range (K), min.	281.44
Temperature range (K), max.	413.94

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=271
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C692966&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
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