3-Heptene, 3-methyl-

Other names:	2-Hexene, 2-ethyl
	3-Methyl-3-heptene
	3-Methyl-3-heptene (c,t)
	3-Methylhept-3-ene
Inchi:	InChI=1S/C8H16/c1-4-6-7-8(3)5-2/h7H,4-6H2,1-3H3/b8-7+
InchiKey:	AAUHUDBDDBJONC-BQYQJAHWSA-N
Formula:	C8H16
SMILES:	CCCC=C(C)CC
Mol. weight [g/mol]:	112.21
CAS:	7300-03-0

Physical Properties

Property code	Value	Unit	Source
gf	88.15	kJ/mol	Joback Method
hf	-101.02	kJ/mol	Joback Method
hfus	15.37	kJ/mol	Joback Method
hvap	33.44	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	784.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	793.00		NIST Webbook
ripol	833.00		NIST Webbook
ripol	833.00		NIST Webbook
ripol	840.00		NIST Webbook
tb	394.15 ± 2.00	K	NIST Webbook
tb	394.25 ± 0.70	K	NIST Webbook
tb	391.65 ± 3.00	K	NIST Webbook
tb	394.35 ± 1.50	K	NIST Webbook
tc	561.75	K	Joback Method
tf	160.88	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.03	J/mol×K	386.48	Joback Method
cpg	231.15	J/mol×K	415.69	Joback Method
cpg	243.70	J/mol×K	444.90	Joback Method
cpg	255.70	J/mol×K	474.11	Joback Method
cpg	267.18	J/mol×K	503.32	Joback Method
cpg	278.15	J/mol×K	532.54	Joback Method
cpg	288.64	J/mol×K	561.75	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49449e+01
Coeff. B	-3.54847e+03
Coeff. C	-5.07240e+01
Temperature range (K), min.	292.82
Temperature range (K), max.	419.07

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7300030&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume