

2-Heptene, 6-methyl-

Other names:	6-Methyl-2-heptene
Inchi:	InChI=1S/C8H16/c1-4-5-6-7-8(2)3/h4-5,8H,6-7H2,1-3H3
InchiKey:	LXBJRNXXTAWCKU-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CC=CCCC(C)C
Mol. weight [g/mol]:	112.21
CAS:	73548-72-8

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	32.97	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
rinpol	787.00		NIST Webbook
tb	390.90 ± 1.00	K	NIST Webbook
tb	390.85 ± 0.50	K	NIST Webbook
tc	562.05	K	Joback Method
tf	159.84	K	Joback Method
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	278.83	J/mol×K	532.73	Joback Method
cpg	267.72	J/mol×K	503.42	Joback Method
cpg	256.10	J/mol×K	474.10	Joback Method
cpg	243.94	J/mol×K	444.79	Joback Method
cpg	231.23	J/mol×K	415.47	Joback Method

cpg	289.43	J/mol×K	562.05	Joback Method
dvisc	0.0001950	Pa×s	386.16	Joback Method
dvisc	0.0002638	Pa×s	348.44	Joback Method
dvisc	0.0003840	Pa×s	310.72	Joback Method
dvisc	0.0006201	Pa×s	273.00	Joback Method
dvisc	0.0011677	Pa×s	235.28	Joback Method
dvisc	0.0028001	Pa×s	197.56	Joback Method
dvisc	0.0101457	Pa×s	159.84	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46383e+01
Coeff. B	-3.44429e+03
Coeff. C	-4.96120e+01
Temperature range (K), min.	289.62
Temperature range (K), max.	418.90

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73548728&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

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

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