

2-Heptene, 6-methyl-, trans

Other names:	(E)-6-Methylhept-2-ene
Inchi:	InChI=1S/C8H16/c1-4-5-6-7-8(2)3/h4-5,8H,6-7H2,1-3H3/b5-4+
InchiKey:	LXBJRNXXTAWCKU-SNAWJCMRSA-N
Formula:	C8H16
SMILES:	CC=CCCC(C)C
Mol. weight [g/mol]:	112.21

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	772.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	771.50		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	768.50		NIST Webbook
rinpol	765.60		NIST Webbook
rinpol	771.50		NIST Webbook
tb	386.16	K	Joback Method
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	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

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R293080&Units=SI

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
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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