

(Z)-3-Heptene

Other names:	3-Heptene, (Z)- CIS-3-HEPTENE
Inchi:	InChI=1S/C7H14/c1-3-5-7-6-4-2/h5,7H,3-4,6H2,1-2H3/b7-5-
InchiKey:	WZHKDGJSXCTSCK-ALCCZGGFSA-N
Formula:	C7H14
SMILES:	CCC=CCCC
Mol. weight [g/mol]:	98.19
CAS:	7642-10-6

Physical Properties

Property code	Value	Unit	Source
gf	88.28	kJ/mol	Joback Method
hf	-69.40	kJ/mol	NIST Webbook
hf	-68.80 ± 0.60	kJ/mol	NIST Webbook
hf	-69.10	kJ/mol	NIST Webbook
hf	-68.50 ± 0.80	kJ/mol	NIST Webbook
hfl	-104.60 ± 0.63	kJ/mol	NIST Webbook
hfl	-104.30 ± 0.79	kJ/mol	NIST Webbook
hfus	14.09	kJ/mol	Joback Method
hvap	35.60	kJ/mol	NIST Webbook
log10ws	-2.61		Crippen Method
logp	2.753		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	690.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	690.40		NIST Webbook
rinpol	691.10		NIST Webbook
rinpol	694.10		NIST Webbook
rinpol	695.30		NIST Webbook
rinpol	697.30		NIST Webbook
rinpol	697.30		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	692.00		NIST Webbook

rinpol	692.00	NIST Webbook
rinpol	697.40	NIST Webbook
rinpol	690.90	NIST Webbook
rinpol	691.00	NIST Webbook
rinpol	692.30	NIST Webbook
rinpol	691.70	NIST Webbook
rinpol	701.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	691.00	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	700.90	NIST Webbook
rinpol	699.00	NIST Webbook
rinpol	701.60	NIST Webbook
rinpol	700.88	NIST Webbook
rinpol	701.00	NIST Webbook
rinpol	701.00	NIST Webbook
rinpol	701.00	NIST Webbook
rinpol	702.00	NIST Webbook
rinpol	701.00	NIST Webbook
rinpol	702.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	701.00	NIST Webbook
rinpol	701.00	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	700.90	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	702.00	NIST Webbook
rinpol	701.00	NIST Webbook
rinpol	691.10	NIST Webbook
rinpol	696.90	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	689.60	NIST Webbook
rinpol	701.10	NIST Webbook
rinpol	696.10	NIST Webbook
rinpol	690.30	NIST Webbook
rinpol	690.50	NIST Webbook
ripol	765.00	NIST Webbook
ripol	756.70	NIST Webbook
ripol	756.20	NIST Webbook
ripol	760.30	NIST Webbook

ripol	756.70		NIST Webbook
ripol	764.00		NIST Webbook
ripol	756.20		NIST Webbook
ripol	760.00		NIST Webbook
ripol	758.00		NIST Webbook
ripol	727.00		NIST Webbook
ripol	757.00		NIST Webbook
ripol	760.30		NIST Webbook
tb	369.00	K	NIST Webbook
tb	368.97 ± 0.30	K	NIST Webbook
tb	369.10 ± 0.50	K	NIST Webbook
tb	369.15 ± 1.00	K	NIST Webbook
tb	368.90 ± 0.30	K	NIST Webbook
tc	536.01	K	Joback Method
tf	163.57	K	Joback Method
vc	0.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.33	J/mol×K	536.01	Joback Method
cpg	233.95	J/mol×K	507.29	Joback Method
cpg	224.15	J/mol×K	478.58	Joback Method
cpg	213.90	J/mol×K	449.86	Joback Method
cpg	203.19	J/mol×K	421.15	Joback Method
cpg	192.00	J/mol×K	392.43	Joback Method
cpg	180.32	J/mol×K	363.72	Joback Method
dvisc	0.0047393	Paxs	163.57	Joback Method
dvisc	0.0001967	Paxs	363.72	Joback Method
dvisc	0.0002558	Paxs	330.36	Joback Method
dvisc	0.0003528	Paxs	297.00	Joback Method
dvisc	0.0005278	Paxs	263.64	Joback Method
dvisc	0.0008875	Paxs	230.29	Joback Method
dvisc	0.0017796	Paxs	196.93	Joback Method
hvapt	35.00	kJ/mol	340.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41650e+01
Coeff. B	-3.13384e+03
Coeff. C	-4.06340e+01
Temperature range (K), min.	266.46
Temperature range (K), max.	394.60

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.14090e+01
Coeff. B	-7.26081e+03
Coeff. C	-1.15726e+01
Coeff. D	9.43755e-06
Temperature range (K), min.	136.51
Temperature range (K), max.	545.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7642106&Units=SI
The Yaws Handbook of Vapor Pressure: KDB Vapor Pressure Data:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=216
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=216

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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