

4-Heptenal, (Z)-

Other names:	cis-4-Hepten-1-al (Z)-4-Hepten-1-al cis-4-Heptenal (4Z)-4-Heptenal 4-(Z)-Heptenal Hept-4(Z)-enal Hept-cis-4-enal (Z)-4-Heptenal (Z)-Hept-4-enal
Inchi:	InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h3-4,7H,2,5-6H2,1H3/b4-3-
InchiKey:	VVGOCOMZRGWHPI-ARJAWSKDSA-N
Formula:	C7H12O
SMILES:	CCC=CCCC=O
Mol. weight [g/mol]:	112.17
CAS:	6728-31-0

Physical Properties

Property code	Value	Unit	Source
gf	-11.24	kJ/mol	Joback Method
hf	-156.17	kJ/mol	Joback Method
hfus	16.38	kJ/mol	Joback Method
hvap	37.85	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpola	898.00		NIST Webbook
rinpola	898.00		NIST Webbook
rinpola	874.00		NIST Webbook
rinpola	902.00		NIST Webbook
rinpola	900.00		NIST Webbook
rinpola	885.00		NIST Webbook
rinpola	901.00		NIST Webbook
rinpola	900.00		NIST Webbook
rinpola	900.00		NIST Webbook
rinpola	900.00		NIST Webbook
rinpola	900.00		NIST Webbook

rinpol	900.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	871.00	NIST Webbook
rinpol	897.00	NIST Webbook
rinpol	901.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	901.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	901.00	NIST Webbook
rinpol	904.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	905.00	NIST Webbook
rinpol	897.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	895.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	904.00	NIST Webbook
rinpol	915.00	NIST Webbook
rinpol	910.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	870.00	NIST Webbook
rinpol	880.00	NIST Webbook
rinpol	879.00	NIST Webbook
rinpol	901.00	NIST Webbook
rinpol	899.10	NIST Webbook
rinpol	871.60	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	902.00	NIST Webbook
rinpol	904.00	NIST Webbook
rinpol	903.00	NIST Webbook
rinpol	902.00	NIST Webbook
rinpol	905.00	NIST Webbook
rinpol	903.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	898.00	NIST Webbook

ripol	888.00	NIST Webbook
ripol	899.00	NIST Webbook
ripol	899.00	NIST Webbook
ripol	900.00	NIST Webbook
ripol	1246.00	NIST Webbook
ripol	1253.00	NIST Webbook
ripol	1263.00	NIST Webbook
ripol	1222.00	NIST Webbook
ripol	1228.00	NIST Webbook
ripol	1218.00	NIST Webbook
ripol	1218.00	NIST Webbook
ripol	1236.00	NIST Webbook
ripol	1230.00	NIST Webbook
ripol	1225.00	NIST Webbook
ripol	1239.00	NIST Webbook
ripol	1234.00	NIST Webbook
ripol	1225.00	NIST Webbook
ripol	1246.00	NIST Webbook
ripol	1247.00	NIST Webbook
ripol	1234.00	NIST Webbook
ripol	1230.00	NIST Webbook
ripol	1244.00	NIST Webbook
ripol	1245.00	NIST Webbook
ripol	1235.00	NIST Webbook
ripol	1247.00	NIST Webbook
ripol	1233.00	NIST Webbook
ripol	1216.00	NIST Webbook
ripol	1255.00	NIST Webbook
ripol	1229.00	NIST Webbook
ripol	1254.00	NIST Webbook
ripol	1246.00	NIST Webbook
ripol	1240.00	NIST Webbook
ripol	1237.00	NIST Webbook
ripol	1260.00	NIST Webbook
ripol	1222.00	NIST Webbook
ripol	1230.00	NIST Webbook
ripol	1245.00	NIST Webbook
ripol	1238.00	NIST Webbook
ripol	1249.00	NIST Webbook
ripol	1260.00	NIST Webbook
ripol	1240.00	NIST Webbook
ripol	1230.00	NIST Webbook
ripol	1219.00	NIST Webbook
ripol	1230.00	NIST Webbook

ripol	1237.00	NIST Webbook
ripol	1260.00	NIST Webbook
ripol	1262.00	NIST Webbook
ripol	1241.00	NIST Webbook
ripol	1250.00	NIST Webbook
ripol	1240.00	NIST Webbook
ripol	1273.00	NIST Webbook
ripol	1269.00	NIST Webbook
ripol	1267.00	NIST Webbook
ripol	1248.00	NIST Webbook
ripol	1246.00	NIST Webbook
ripol	1239.00	NIST Webbook
ripol	1251.00	NIST Webbook
ripol	1251.00	NIST Webbook
ripol	1249.00	NIST Webbook
ripol	1246.00	NIST Webbook
ripol	1221.00	NIST Webbook
ripol	1223.00	NIST Webbook
ripol	1257.00	NIST Webbook
ripol	1238.00	NIST Webbook
ripol	1236.00	NIST Webbook
ripol	1238.00	NIST Webbook
ripol	1236.00	NIST Webbook
ripol	1233.00	NIST Webbook
ripol	1240.00	NIST Webbook
ripol	1254.00	NIST Webbook
ripol	1248.00	NIST Webbook
ripol	1237.00	NIST Webbook
ripol	1243.00	NIST Webbook
ripol	1239.00	NIST Webbook
ripol	1229.00	NIST Webbook
ripol	1229.00	NIST Webbook
ripol	1267.00	NIST Webbook
ripol	1253.00	NIST Webbook
ripol	1251.00	NIST Webbook
ripol	1255.00	NIST Webbook
ripol	1246.00	NIST Webbook
ripol	1246.00	NIST Webbook
ripol	1253.00	NIST Webbook
ripol	1247.00	NIST Webbook
ripol	1231.00	NIST Webbook
ripol	1231.00	NIST Webbook
ripol	1216.00	NIST Webbook
ripol	1233.00	NIST Webbook

ripol	1220.00		NIST Webbook
ripol	1234.00		NIST Webbook
ripol	1242.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1247.00		NIST Webbook
ripol	1236.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1237.00		NIST Webbook
ripol	1247.00		NIST Webbook
ripol	1235.00		NIST Webbook
ripol	1216.00		NIST Webbook
ripol	1237.00		NIST Webbook
ripol	1247.00		NIST Webbook
tb	412.38	K	Joback Method
tc	592.75	K	Joback Method
tf	205.57	K	Joback Method
vc	0.424	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.75	J/molxK	412.38	Joback Method
cpg	212.47	J/molxK	442.44	Joback Method
cpg	222.70	J/molxK	472.50	Joback Method
cpg	232.44	J/molxK	502.57	Joback Method
cpg	241.72	J/molxK	532.63	Joback Method
cpg	250.55	J/molxK	562.69	Joback Method
cpg	258.96	J/molxK	592.75	Joback Method
dvisc	0.0042661	Paxs	205.57	Joback Method
dvisc	0.0019261	Paxs	240.04	Joback Method
dvisc	0.0010618	Paxs	274.51	Joback Method
dvisc	0.0006685	Paxs	308.98	Joback Method
dvisc	0.0004619	Paxs	343.44	Joback Method
dvisc	0.0003414	Paxs	377.91	Joback Method
dvisc	0.0002654	Paxs	412.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6728310&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/38-301-5/4-Heptenal-Z.pdf>

Generated by Cheméo on 2024-04-24 14:09:27.969864748 +0000 UTC m=+16257016.890442063.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.