

2-Heptenal, (E)-

Other names:	(E)-2-Hepten-1-al
	(E)-2-Heptenal
	n-Hept-trans-2-enal
	trans-2-Heptenal
	Hept-trans-2-enal
	2-trans-Heptenal
	trans-2-Hepten-1-al
	«beta»-Butylacrolein
	3-Butylacrolein
	(2E)-2-Heptenal
	(2E)-Heptenal
	(E)-hept-2-enal
	Hept-2(E)-enal
	Hept-(E)-2-enal
	2-Heptenal, (2E)-
Inchi:	InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h5-7H,2-4H2,1H3/b6-5+
InchiKey:	NDFKTBCGKNOHPJ-AATRIKPKSA-N
Formula:	C7H12O
SMILES:	CCCCC=CC=O
Mol. weight [g/mol]:	112.17
CAS:	18829-55-5

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
rinpol	960.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	953.00		NIST Webbook

rinpol	959.00	NIST Webbook
rinpol	934.00	NIST Webbook
rinpol	967.00	NIST Webbook
rinpol	954.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	946.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	967.00	NIST Webbook
rinpol	940.00	NIST Webbook
rinpol	934.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	978.00	NIST Webbook
rinpol	978.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	947.00	NIST Webbook
rinpol	956.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	929.00	NIST Webbook
rinpol	928.00	NIST Webbook
rinpol	932.00	NIST Webbook
rinpol	931.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	963.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	953.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	924.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	934.00	NIST Webbook
rinpol	931.00	NIST Webbook
rinpol	929.00	NIST Webbook
rinpol	953.00	NIST Webbook
rinpol	954.00	NIST Webbook

rinpol	964.00	NIST Webbook
rinpol	953.00	NIST Webbook
rinpol	956.00	NIST Webbook
rinpol	955.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	959.00	NIST Webbook
rinpol	956.00	NIST Webbook
rinpol	952.00	NIST Webbook
rinpol	931.00	NIST Webbook
rinpol	954.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	956.00	NIST Webbook
rinpol	956.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	964.00	NIST Webbook
rinpol	934.00	NIST Webbook
rinpol	955.00	NIST Webbook
rinpol	953.00	NIST Webbook
rinpol	956.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	951.00	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	956.00	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	954.00	NIST Webbook
rinpol	930.00	NIST Webbook
rinpol	972.00	NIST Webbook
rinpol	968.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	978.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	940.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	954.00	NIST Webbook
rinpol	953.00	NIST Webbook
rinpol	931.00	NIST Webbook
rinpol	932.00	NIST Webbook
rinpol	923.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	937.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	930.00	NIST Webbook

rinpol	957.00	NIST Webbook
rinpol	930.00	NIST Webbook
rinpol	964.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	975.00	NIST Webbook
rinpol	978.00	NIST Webbook
rinpol	923.00	NIST Webbook
rinpol	978.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	929.00	NIST Webbook
rinpol	952.00	NIST Webbook
rinpol	941.00	NIST Webbook
rinpol	941.00	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	959.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	955.00	NIST Webbook
rinpol	942.00	NIST Webbook
rinpol	967.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	956.00	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	954.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	926.00	NIST Webbook
rinpol	931.00	NIST Webbook
rinpol	957.00	NIST Webbook
ripol	1334.00	NIST Webbook
ripol	1315.00	NIST Webbook
ripol	1321.00	NIST Webbook
ripol	1303.00	NIST Webbook
ripol	1332.00	NIST Webbook
ripol	1309.00	NIST Webbook
ripol	1366.00	NIST Webbook
ripol	1324.00	NIST Webbook
ripol	1313.00	NIST Webbook
ripol	1320.00	NIST Webbook
ripol	1335.00	NIST Webbook
ripol	1310.00	NIST Webbook
ripol	1312.00	NIST Webbook
ripol	1328.00	NIST Webbook
ripol	1315.00	NIST Webbook
ripol	1316.00	NIST Webbook
ripol	1287.00	NIST Webbook

ripol	1320.00	NIST Webbook
ripol	1335.00	NIST Webbook
ripol	1335.00	NIST Webbook
ripol	1335.00	NIST Webbook
ripol	1335.00	NIST Webbook
ripol	1335.00	NIST Webbook
ripol	1335.00	NIST Webbook
ripol	1335.00	NIST Webbook
ripol	1339.00	NIST Webbook
ripol	1318.00	NIST Webbook
ripol	1329.00	NIST Webbook
ripol	1315.00	NIST Webbook
ripol	1334.00	NIST Webbook
ripol	1334.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1314.00	NIST Webbook
ripol	1286.00	NIST Webbook
ripol	1315.00	NIST Webbook
ripol	1313.00	NIST Webbook
ripol	1315.00	NIST Webbook
ripol	1313.00	NIST Webbook
ripol	1323.00	NIST Webbook
ripol	1321.00	NIST Webbook
ripol	1320.00	NIST Webbook
ripol	1320.00	NIST Webbook
ripol	1317.00	NIST Webbook
ripol	1314.00	NIST Webbook
ripol	1303.00	NIST Webbook
ripol	1317.00	NIST Webbook
ripol	1314.00	NIST Webbook
ripol	1321.00	NIST Webbook
ripol	1321.00	NIST Webbook
ripol	1332.00	NIST Webbook
ripol	1313.00	NIST Webbook
ripol	1321.00	NIST Webbook
ripol	1292.00	NIST Webbook
ripol	1320.00	NIST Webbook
ripol	1309.00	NIST Webbook
ripol	1328.00	NIST Webbook
ripol	1336.00	NIST Webbook
ripol	1297.00	NIST Webbook
ripol	1297.00	NIST Webbook
ripol	1366.00	NIST Webbook

ripol	1362.00		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1346.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1273.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1314.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1306.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1321.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1320.00		NIST Webbook
tb	412.38	K	Joback Method
tc	592.75	K	Joback Method

tf	205.57	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	363.70	K	6.70	NIST Webbook

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=C18829555&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/69-094-2/2-Heptenal-E.pdf>

Generated by Cheméo on 2025-12-05 08:27:52.609854423 +0000 UTC m=+4671470.139895076.

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