

Hexane, 1-iodo-

Other names:	1-Hexyl iodide 1-Iodohexane Hexyl iodide N-HEXYL IODIDE n-C6H13I
Inchi:	InChI=1S/C6H13I/c1-2-3-4-5-6-7/h2-6H2,1H3
InchiKey:	ANOOTOPTCJRUPK-UHFFFAOYSA-N
Formula:	C6H13I
SMILES:	CCCCCCI
Mol. weight [g/mol]:	212.07
CAS:	638-45-9

Physical Properties

Property code	Value	Unit	Source
gf	57.76	kJ/mol	Joback Method
hf	-90.30	kJ/mol	Joback Method
hfus	15.70	kJ/mol	Joback Method
hvap	49.80 ± 0.10	kJ/mol	NIST Webbook
hvap	49.75 ± 0.08	kJ/mol	NIST Webbook
hvap	49.76	kJ/mol	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.13	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-3.28		Crippen Method
logp	3.002		Crippen Method
mcvol	121.220	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1011.80		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1032.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1257.00		NIST Webbook

ripol	1275.00		NIST Webbook
ripol	1272.00		NIST Webbook
tb	349.65	K	KDB
tb	454.50	K	NIST Webbook
tb	452.70	K	NIST Webbook
tc	630.19	K	Joback Method
tf	198.95 ± 0.60	K	NIST Webbook
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.87	J/mol×K	630.19	Joback Method
cpg	231.02	J/mol×K	496.61	Joback Method
cpg	220.55	J/mol×K	463.22	Joback Method
cpg	240.96	J/mol×K	530.01	Joback Method
cpg	250.40	J/mol×K	563.40	Joback Method
cpg	259.36	J/mol×K	596.80	Joback Method
cpg	209.53	J/mol×K	429.82	Joback Method
cpl	224.16	J/mol×K	318.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	216.53	J/mol×K	293.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition

cpl	217.80	J/mol×K	298.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	220.77	J/mol×K	308.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	222.46	J/mol×K	313.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	219.28	J/mol×K	303.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	225.86	J/mol×K	323.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition

cpl	227.13	J/mol×K	328.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	227.98	J/mol×K	333.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	229.04	J/mol×K	338.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	229.89	J/mol×K	343.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	232.64	J/mol×K	353.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	222.50	J/mol×K	298.15	NIST Webbook

cpl	234.34	J/mol×K	358.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	236.04	J/mol×K	363.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	237.52	J/mol×K	368.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	238.79	J/mol×K	373.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	231.16	J/mol×K	348.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
dvisc	0.0062823	Pa×s	215.44	Joback Method
dvisc	0.0027872	Pa×s	251.17	Joback Method
dvisc	0.0015140	Pa×s	286.90	Joback Method

dvisc	0.0009414	Pa×s	322.63	Joback Method
dvisc	0.0006436	Pa×s	358.36	Joback Method
dvisc	0.0003636	Pa×s	429.82	Joback Method
dvisc	0.0004714	Pa×s	394.09	Joback Method
hvapt	46.20	kJ/mol	408.00	NIST Webbook
kvisc	0.0000005	m2/s	348.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000004	m2/s	383.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000004	m2/s	368.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000005	m2/s	358.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000004	m2/s	393.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000003	m2/s	413.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K

kvisc	0.0000006	m2/s	338.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000003	m2/s	423.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000006	m2/s	333.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000006	m2/s	328.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000007	m2/s	323.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000007	m2/s	318.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000009	m2/s	300.25	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K

kvisc	0.0000009	m2/s	298.25	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000009	m2/s	298.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000009	m2/s	297.25	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000007	m2/s	319.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000005	m2/s	343.15	Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
pvap	0.08	kPa	288.15	Vapor Pressure of Selected Organic Iodides
pvap	6.84e-03	kPa	258.17	Vapor Pressure of Selected Organic Iodides
pvap	6.85e-03	kPa	258.18	Vapor Pressure of Selected Organic Iodides
pvap	6.85e-03	kPa	258.18	Vapor Pressure of Selected Organic Iodides
pvap	0.01	kPa	263.17	Vapor Pressure of Selected Organic Iodides

pvap	0.01	kPa	263.17	Vapor Pressure of Selected Organic Iodides
pvap	0.01	kPa	263.17	Vapor Pressure of Selected Organic Iodides
pvap	0.02	kPa	268.17	Vapor Pressure of Selected Organic Iodides
pvap	0.02	kPa	268.17	Vapor Pressure of Selected Organic Iodides
pvap	0.02	kPa	268.17	Vapor Pressure of Selected Organic Iodides
pvap	0.03	kPa	273.65	Vapor Pressure of Selected Organic Iodides
pvap	0.03	kPa	273.65	Vapor Pressure of Selected Organic Iodides
pvap	0.04	kPa	278.15	Vapor Pressure of Selected Organic Iodides
pvap	0.04	kPa	278.15	Vapor Pressure of Selected Organic Iodides
pvap	0.06	kPa	283.15	Vapor Pressure of Selected Organic Iodides
pvap	0.06	kPa	283.15	Vapor Pressure of Selected Organic Iodides
pvap	0.32	kPa	308.15	Vapor Pressure of Selected Organic Iodides
pvap	0.32	kPa	308.15	Vapor Pressure of Selected Organic Iodides
pvap	0.32	kPa	308.15	Vapor Pressure of Selected Organic Iodides
pvap	0.24	kPa	303.15	Vapor Pressure of Selected Organic Iodides
pvap	0.24	kPa	303.15	Vapor Pressure of Selected Organic Iodides
pvap	0.17	kPa	298.15	Vapor Pressure of Selected Organic Iodides
pvap	0.17	kPa	298.15	Vapor Pressure of Selected Organic Iodides
pvap	0.12	kPa	293.15	Vapor Pressure of Selected Organic Iodides

pvap	0.12	kPa	293.15	Vapor Pressure of Selected Organic Iodides	
pvap	0.08	kPa	288.15	Vapor Pressure of Selected Organic Iodides	
pvap	0.03	kPa	273.65	Vapor Pressure of Selected Organic Iodides	
speedsl	1045.50	m/s	293.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohexane, and 1-Chlorohexane + 1-Iodohexane at Saturation Condition	
speedsl	1017.20	m/s	303.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohexane, and 1-Chlorohexane + 1-Iodohexane at Saturation Condition	
speedsl	1003.20	m/s	308.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohexane, and 1-Chlorohexane + 1-Iodohexane at Saturation Condition	
speedsl	989.20	m/s	313.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohexane, and 1-Chlorohexane + 1-Iodohexane at Saturation Condition	
speedsl	828.00	m/s	373.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohexane, and 1-Chlorohexane + 1-Iodohexane at Saturation Condition	

speedsl	841.00	m/s	368.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohehexane, and 1-Chlorohexane + 1-Iodohehexane at Saturation Condition
speedsl	1031.30	m/s	298.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohehexane, and 1-Chlorohexane + 1-Iodohehexane at Saturation Condition
speedsl	854.10	m/s	363.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohehexane, and 1-Chlorohexane + 1-Iodohehexane at Saturation Condition
speedsl	867.30	m/s	358.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohehexane, and 1-Chlorohexane + 1-Iodohehexane at Saturation Condition
speedsl	880.50	m/s	353.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohehexane, and 1-Chlorohexane + 1-Iodohehexane at Saturation Condition
speedsl	893.80	m/s	348.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohehexane, and 1-Chlorohexane + 1-Iodohehexane at Saturation Condition

speedsl	907.20	m/s	343.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohexane, and 1-Chlorohexane + 1-Iodohexane at Saturation Condition
speedsl	920.70	m/s	338.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohexane, and 1-Chlorohexane + 1-Iodohexane at Saturation Condition
speedsl	934.20	m/s	333.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohexane, and 1-Chlorohexane + 1-Iodohexane at Saturation Condition
speedsl	947.90	m/s	328.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohexane, and 1-Chlorohexane + 1-Iodohexane at Saturation Condition
speedsl	961.60	m/s	323.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohexane, and 1-Chlorohexane + 1-Iodohexane at Saturation Condition
speedsl	975.40	m/s	318.15	Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodohexane, and 1-Chlorohexane + 1-Iodohexane at Saturation Condition

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49062e+01
Coeff. B	-3.96294e+03
Coeff. C	-6.74950e+01
Temperature range (K), min.	338.58
Temperature range (K), max.	480.53

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.00406e+02
Coeff. B	-9.28950e+03
Coeff. C	-1.25591e+01
Coeff. D	7.27406e-06
Temperature range (K), min.	331.15
Temperature range (K), max.	485.15

Datasets

Speed of sound, m/s

Temperature, K - Liquid	Pressure, kPa - Liquid	Speed of sound, m/s - Liquid
293.15	100.00	1045.5
293.15	5000.00	1064.5
293.15	10000.00	1082.0
293.15	20000.00	1113.9
293.15	30000.00	1144.3
293.15	40000.00	1172.4
293.15	50000.00	1198.8
293.15	60000.00	1224.5
293.15	70000.00	1248.5

293.15	80000.00	1272.5
293.15	90000.00	1295.5
293.15	100000.00	1318.0
293.15	110000.00	1339.6
293.15	120000.00	1361.6
293.15	130000.00	1383.8
293.15	140000.00	1403.0
293.15	150000.00	1422.2
293.15	160000.00	1441.0
293.15	170000.00	1458.3
293.15	180000.00	1473.8
293.15	190000.00	1486.4
293.15	200000.00	1498.6
313.15	100.00	989.2
313.15	5000.00	1008.1
313.15	10000.00	1026.8
313.15	20000.00	1061.9
313.15	30000.00	1094.5
313.15	40000.00	1124.9
313.15	50000.00	1153.5
313.15	60000.00	1180.6
313.15	70000.00	1206.3
313.15	80000.00	1231.0
313.15	90000.00	1254.8
313.15	100000.00	1277.7
313.15	110000.00	1300.0
313.15	120000.00	1321.6
313.15	130000.00	1342.6
313.15	140000.00	1363.0
313.15	150000.00	1382.7
313.15	160000.00	1401.6
313.15	170000.00	1419.6
313.15	180000.00	1436.5
313.15	190000.00	1452.0
313.15	200000.00	1466.0
333.15	100.00	934.2
333.15	5000.00	954.9
333.15	10000.00	974.8
333.15	20000.00	1012.2
333.15	30000.00	1046.7
333.15	40000.00	1078.7
333.15	50000.00	1108.8
333.15	60000.00	1137.0
333.15	70000.00	1163.8

333.15	80000.00	1189.4
333.15	90000.00	1214.0
333.15	100000.00	1237.7
333.15	110000.00	1260.6
333.15	120000.00	1282.9
333.15	130000.00	1304.5
333.15	140000.00	1325.5
333.15	150000.00	1345.8
333.15	160000.00	1365.3
333.15	170000.00	1383.9
333.15	180000.00	1401.5
333.15	190000.00	1417.7
333.15	200000.00	1432.3
353.15	100.00	880.5
353.15	5000.00	901.4
353.15	10000.00	922.9
353.15	20000.00	963.3
353.15	30000.00	1000.4
353.15	40000.00	1034.7
353.15	50000.00	1066.6
353.15	60000.00	1096.4
353.15	70000.00	1124.4
353.15	80000.00	1151.0
353.15	90000.00	1176.3
353.15	100000.00	1200.6
353.15	110000.00	1224.1
353.15	120000.00	1246.8
353.15	130000.00	1268.9
353.15	140000.00	1290.4
353.15	150000.00	1311.4
353.15	160000.00	1331.8
353.15	170000.00	1351.7
353.15	180000.00	1370.8
353.15	190000.00	1389.1
353.15	200000.00	1406.5
373.15	100.00	828.0
373.15	5000.00	849.1
373.15	10000.00	872.1
373.15	20000.00	915.3
373.15	30000.00	955.2
373.15	40000.00	992.0
373.15	50000.00	1026.1
373.15	60000.00	1057.9
373.15	70000.00	1087.6

373.15	80000.00	1115.5
373.15	90000.00	1141.9
373.15	100000.00	1166.9
373.15	110000.00	1190.8
373.15	120000.00	1213.8
373.15	130000.00	1236.0
373.15	140000.00	1257.4
373.15	150000.00	1278.2
373.15	160000.00	1298.6
373.15	170000.00	1318.3
373.15	180000.00	1337.6
373.15	190000.00	1356.4
373.15	200000.00	1374.6
393.15	100.00	776.7
393.15	5000.00	802.4
393.15	10000.00	827.2
393.15	20000.00	873.1
393.15	30000.00	914.8
393.15	40000.00	959.9
393.15	50000.00	988.0
393.15	60000.00	1020.6
393.15	70000.00	1051.2
393.15	80000.00	1080.1
393.15	90000.00	1107.6
393.15	100000.00	1133.9
393.15	110000.00	1159.1
393.15	120000.00	1183.3
393.15	130000.00	1206.4
393.15	140000.00	1228.7
393.15	150000.00	1249.0
393.15	160000.00	1267.9
393.15	170000.00	1292.2
393.15	180000.00	1307.3
393.15	190000.00	1327.4
393.15	200000.00	1342.7
413.15	100.00	725.6
413.15	5000.00	753.2
413.15	10000.00	779.8
413.15	20000.00	828.6
413.15	30000.00	872.6
413.15	40000.00	912.5
413.15	50000.00	949.2
413.15	60000.00	983.3
413.15	70000.00	1015.2

413.15	80000.00	1045.3
413.15	90000.00	1073.9
413.15	100000.00	1101.0
413.15	110000.00	1126.6
413.15	120000.00	1152.7
413.15	130000.00	1177.1
413.15	140000.00	1200.6
413.15	150000.00	1223.2
413.15	160000.00	1244.7
413.15	170000.00	1266.0
413.15	180000.00	1283.2
413.15	190000.00	1298.6
413.15	200000.00	1314.1

Reference

<https://www.doi.org/10.1021/je050069s>

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Chloroheptane, and 1-Chlorononane at Saturation Condition:

<https://www.doi.org/10.1021/je034013e>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Speed of Sound of Hexane +

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1636>

1-Chlorohexane, Hexane +

<https://www.doi.org/10.1021/je0256129>

Joback Method: 1-Iodoheptane, and 1-Chlorohexane + 1-Iodoheptane at Saturation Condition: Vapor Pressure of Selected Organic Iodides:

https://en.wikipedia.org/wiki/Joback_method

<https://www.doi.org/10.1021/je100398m>

Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition:

<https://www.doi.org/10.1021/je060158k>

<https://www.doi.org/10.1021/je050069s>

Speed of Sound of Hexane + 1-Chlorohexane, Hexane + 1-Iodoheptane, and 1-Chlorohexane + 1-Iodoheptane at Temperatures from (293.15 to 413.15) K and Pressures up to 200 MPa:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C638459&Units=SI>

<https://www.thermo.com/files/research/kdb/mol/mol1636.mol>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Legend

cp _g :	Ideal gas heat capacity
cp _l :	Liquid phase heat capacity
dv _{isc} :	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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
kvisc:	Kinematic viscosity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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