

Heptane, 1-iodo-

Other names:	1-Iodoheptane 1-Iodomeptane Heptyl iodide n-Heptyl iodide
Inchi:	InChI=1S/C7H15I/c1-2-3-4-5-6-7-8/h2-7H2,1H3
InchiKey:	LMHCYRULPLGEEZ-UHFFFAOYSA-N
Formula:	C7H15I
SMILES:	CCCCCCI
Mol. weight [g/mol]:	226.10
CAS:	4282-40-0

Physical Properties

Property code	Value	Unit	Source
gf	66.18	kJ/mol	Joback Method
hf	-110.94	kJ/mol	Joback Method
hfus	18.29	kJ/mol	Joback Method
hvap	55.00	kJ/mol	NIST Webbook
log10ws	-4.81		Aqueous Solubility Prediction Method
log10ws	-4.81		Estimated Solubility Method
logp	3.392		Crippen Method
mcvol	135.310	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	1114.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1122.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1353.00		NIST Webbook
tb	477.20	K	NIST Webbook

tc	650.84	K	Joback Method
tf	225.08	K	Aqueous Solubility Prediction Method
vc	0.515	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.07	J/mol×K	650.84	Joback Method
cpg	261.42	J/mol×K	485.72	Joback Method
cpg	273.06	J/mol×K	518.75	Joback Method
cpg	284.11	J/mol×K	551.77	Joback Method
cpg	294.62	J/mol×K	584.79	Joback Method
cpg	304.59	J/mol×K	617.82	Joback Method
cpg	249.19	J/mol×K	452.70	Joback Method
cpl	261.82	J/mol×K	328.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	263.40	J/mol×K	333.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	264.99	J/mol×K	338.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition

cpl	266.80	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	267.93	J/mol×K	348.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	260.01	J/mol×K	323.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	271.32	J/mol×K	358.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	273.13	J/mol×K	363.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition

cpl	274.71	J/molxK	368.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	276.52	J/molxK	373.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	251.80	J/molxK	298.15	NIST Webbook
cpl	257.98	J/molxK	318.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	256.17	J/molxK	313.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	254.13	J/molxK	308.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition

cpl	252.33	J/mol×K	303.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	249.84	J/mol×K	298.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	269.96	J/mol×K	353.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
cpl	246.90	J/mol×K	293.15	Temperature Dependence of the Thermophysical Properties of 1-Chlorohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition
dvisc	0.0006070	Paxs	377.37	Joback Method
dvisc	0.0062596	Paxs	226.71	Joback Method
dvisc	0.0003384	Paxs	452.70	Joback Method
dvisc	0.0027223	Paxs	264.38	Joback Method
dvisc	0.0014572	Paxs	302.04	Joback Method
dvisc	0.0008959	Paxs	339.71	Joback Method
dvisc	0.0004414	Paxs	415.04	Joback Method
hvapt	47.80	kJ/mol	443.00	NIST Webbook

kvisc	0.0000005	m2/s	368.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000007	m2/s	338.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000007	m2/s	343.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000006	m2/s	348.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000006	m2/s	353.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000005	m2/s	363.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000007	m2/s	333.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K

kvisc	0.0000005	m2/s	373.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000005	m2/s	378.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000005	m2/s	383.15	Kinematic Viscosity of 1-Iodoheptane, 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-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000004	m2/s	403.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000004	m2/s	413.15	Kinematic Viscosity of 1-Iodoheptane, 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-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K

kvisc	0.0000008	m2/s	328.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000008	m2/s	323.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000009	m2/s	318.15	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000009	m2/s	313.20	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000011	m2/s	303.50	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000012	m2/s	296.35	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K
kvisc	0.0000012	m2/s	297.20	Kinematic Viscosity of 1-Iodoheptane, 1-Iodoheptane, and 1-Chlorononane at Temperatures from (293.15 to 423.15) K

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47838e+01
Coeff. B	-4.10093e+03
Coeff. C	-7.37840e+01
Temperature range (K), min.	356.68
Temperature range (K), max.	506.72

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4282400&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Kinematic Viscosity of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Temperatures From (293.15 to 423.15) K:	https://www.doi.org/10.1021/je060158k
Temperature Dependence of the Thermophysical Properties of 1-Iodohexane, 1-Iodoheptane, and 1-Chlorononane at Saturation Condition:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	https://www.doi.org/10.1021/je034013e
Gruppen Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
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
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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