Pentane, 1-iodo-

Other names:	1-Iodopentane
	1-Jodpentan
	1-Pentyl iodide
	Amyl iodide
	N-AMYL IODIDE
	N-PENTYL IODIDE
	NSC 7901
	Pentyl iodide
	n-C5H11I
Inchi:	InChI=1S/C5H11I/c1-2-3-4-5-6/h2-5H2,1H3
InchiKey:	BLXSFCHWMBESKV-UHFFFAOYSA-N
Formula:	C5H11I
SMILES:	CCCCCI
Mol. weight [g/mol]:	198.05
CAS:	628-17-1

Physical Properties

Property code	Value	Unit	Source
gf	49.34	kJ/mol	Joback Method
hf	-69.66	kJ/mol	Joback Method
hfus	13.11	kJ/mol	Joback Method
hvap	44.40	kJ/mol	NIST Webbook
hvap	45.30 ± 0.10	kJ/mol	NIST Webbook
hvap	45.27 ± 0.02	kJ/mol	NIST Webbook
hvap	45.27	kJ/mol	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.18 ± 0.01	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
ie	9.21	eV	NIST Webbook
ie	9.21	eV	NIST Webbook
ie	9.19 ± 0.01	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.20 ± 0.01	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.86		Crippen Method
logp	2.612		Crippen Method

mcvol	107.130	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	903.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	917.80		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	912.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1175.00		NIST Webbook
ripol	1166.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1160.00		NIST Webbook
tb	419.70 ± 0.60	K	NIST Webbook
tb	428.00	K	NIST Webbook
tb	430.15	K	KDB
tb	427.70	K	NIST Webbook
tb	430.20	K	NIST Webbook
tc	609.36	K	Joback Method
tf	187.55	K	KDB
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.12	J/mol×K	406.94	Joback Method
cpg	223.14	J/mol×K	609.36	Joback Method
cpg	215.72	J/mol×K	575.63	Joback Method
cpg	207.88	J/mol×K	541.89	Joback Method
cpg	199.63	J/mol×K	508.15	Joback Method
cpg	190.93	J/mol×K	474.41	Joback Method
cpg	181.77	J/mol×K	440.68	Joback Method
cpl	193.60	J/mol×K	298.15	NIST Webbook
dvisc	0.0028062	Pa×s	237.96	Joback Method
dvisc	0.0003861	Pa×s	406.94	Joback Method
dvisc	0.0004973	Pa×s	373.14	Joback Method
dvisc	0.0006735	Pa×s	339.35	Joback Method
dvisc	0.0009755	Pa×s	305.56	Joback Method
dvisc	0.0015494	Pa×s	271.76	Joback Method
dvisc	0.0061872	Pa×s	204.17	Joback Method
hvapt	43.10	kJ/mol	392.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49242e+01
Coeff. B	-3.78193e+03
Coeff. C	-6.07320e+01
Temperature range (K), min.	319.12
Temperature range (K), max.	454.16

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.41903e+01
Coeff. B	-8.49587e+03
Coeff. C	-1.17381e+01
Coeff. D	7.34893e-06
Temperature range (K), min.	312.15
Temperature range (K), max.	473.15

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1625.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C628171&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1625

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

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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