1-Propene, 3-iodo-

Other names:	2-Propene, 1-iodo
	3-IODOPROPYLENE
	3-Iodo-1-propene
	3-Iodopropene
	ALLYL IODIDE
	CH2CHCH2I
	Propene, 3-iodo-
	UN 1723
Inchi:	InChI=1S/C3H5I/c1-2-3-4/h2H,1,3H2
InchiKey:	HFEHLDPGIKPNKL-UHFFFAOYSA-N
Formula:	C3H5I
SMILES:	C=CCI
Mol. weight [g/mol]:	167.98
CAS:	556-56-9

Physical Properties

Property code	Value	Unit	Source
af	0.2020		KDB
gf	120.34	kJ/mol	Joback Method
hf	93.30 ± 6.30	kJ/mol	NIST Webbook
hf	89.80 ± 1.40	kJ/mol	NIST Webbook
hf	99.50	kJ/mol	NIST Webbook
hfl	55.20 ± 5.40	kJ/mol	NIST Webbook
hfus	6.65	kJ/mol	Joback Method
hvap	38.00 ± 2.00	kJ/mol	NIST Webbook
ie	9.32	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.37	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.27	eV	NIST Webbook
log10ws	-1.88		Crippen Method
logp	1.607		Crippen Method
mcvol	74.650	ml/mol	McGowan Method
pc	4530.00	kPa	KDB
rinpol	687.00		NIST Webbook

rinpol	688.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	688.00		NIST Webbook
tb	375.00 ± 1.00	K	NIST Webbook
tb	375.00	K	NIST Webbook
tb	374.95 ± 0.35	K	NIST Webbook
tb	375.20	K	KDB
tb	376.20	K	NIST Webbook
tc	595.80	K	KDB
tf	173.90 ± 0.50	K	NIST Webbook
tf	176.00 ± 0.50	K	NIST Webbook
tf	174.00	K	KDB
vc	0.273	m3/kmol	KDB
zc	0.2491880		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.55	J/mol×K	357.86	Joback Method
cpg	97.14	J/mol×K	392.94	Joback Method
cpg	102.37	J/mol×K	428.02	Joback Method
cpg	107.26	J/mol×K	463.10	Joback Method
cpg	111.83	J/mol×K	498.18	Joback Method
cpg	116.10	J/mol×K	533.26	Joback Method
cpg	120.09	J/mol×K	568.34	Joback Method
dvisc	0.0046445	Pa×s	179.87	Joback Method
dvisc	0.0023176	Pa×s	209.53	Joback Method
dvisc	0.0013741	Pa×s	239.20	Joback Method
dvisc	0.0009143	Pa×s	268.87	Joback Method
dvisc	0.0006597	Pa×s	298.53	Joback Method
dvisc	0.0005049	Pa×s	328.20	Joback Method
dvisc	0.0004039	Pa×s	357.86	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.55144e+01
Coeff. B	-3.60393e+03
Coeff. C	-4.54440e+01
Temperature range (K), min.	282.13
Temperature range (K), max.	398.67

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.85269e+01
Coeff. B	-7.03924e+03
Coeff. C	-9.43675e+00
Coeff. D	5.62626e-06
Temperature range (K), min.	293.15
Temperature range (K), max.	595.81

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C556569&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=1741

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1741.mol

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility