Propane, 1-iodo-2,2-dimethyl-

Other names:	1-Iodo-2,2-dimethylpropane
	2,2-Dimethyl-1-iodopropane
	2,2-Dimethylpropyl iodide
	Neopentyl iodide
Inchi:	InChI=1S/C5H11I/c1-5(2,3)4-6/h4H2,1-3H3
InchiKey:	CJTZXIJETZZARD-UHFFFAOYSA-N
Formula:	C5H11I
SMILES:	CC(C)(C)CI
Mol. weight [g/mol]:	198.05
CAS:	15501-33-4

Physical Properties

Property code	Value	Unit	Source
gf	52.18	kJ/mol	Joback Method
hf	-78.41	kJ/mol	Joback Method
hfus	5.70	kJ/mol	Joback Method
hvap	34.80	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.468		Crippen Method
mcvol	107.130	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	403.71	K	Joback Method
tc	620.61	K	Joback Method
tf	206.59	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.23	J/mol×K	403.71	Joback Method
cpg	222.44	J/mol×K	584.46	Joback Method
cpg	214.14	J/mol×K	548.31	Joback Method
cpg	205.21	J/mol×K	512.16	Joback Method
cpg	195.61	J/mol×K	476.01	Joback Method

cpg	185.30	J/mol×K	439.86	Joback Method
cpg	230.17	J/mol×K	620.61	Joback Method
dvisc	0.0004201	Pa×s	403.71	Joback Method
dvisc	0.0005683	Pa×s	370.86	Joback Method
dvisc	0.0008153	Pa×s	338.00	Joback Method
dvisc	0.0012642	Pa×s	305.15	Joback Method
dvisc	0.0021792	Pa×s	272.30	Joback Method
dvisc	0.0043620	Pa×s	239.44	Joback Method
dvisc	0.0108874	Pa×s	206.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.70	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30430e+01
Coeff. B	-3.14272e+03
Coeff. C	-5.43380e+01
Temperature range (K), min.	300.72
Temperature range (K), max.	460.82

Sources

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=C15501334&Units=SI

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume