

Propane, 1-chloro-3-iodo-

Other names:	1-Chloro-3-iodopropane 3-Chloropropyl iodide
Inchi:	InChI=1S/C3H6ClI/c4-2-1-3-5/h1-3H2
InchiKey:	SFOYQZYQTQDRYI-UHFFFAOYSA-N
Formula:	C3H6ClI
SMILES:	CICCCI
Mol. weight [g/mol]:	204.44
CAS:	6940-76-7

Physical Properties

Property code	Value	Unit	Source
gf	20.57	kJ/mol	Joback Method
hf	-44.12	kJ/mol	Joback Method
hfus	12.13	kJ/mol	Joback Method
hvap	36.03	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.050		Crippen Method
mvol	91.190	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	444.20	K	NIST Webbook
tc	613.31	K	Joback Method
tf	211.55	K	Joback Method
vc	0.341	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.44	J/molxK	398.61	Joback Method
cpg	130.59	J/molxK	434.39	Joback Method
cpg	136.37	J/molxK	470.18	Joback Method
cpg	141.80	J/molxK	505.96	Joback Method
cpg	146.89	J/molxK	541.74	Joback Method
cpg	151.67	J/molxK	577.53	Joback Method
cpg	156.16	J/molxK	613.31	Joback Method

dvisc	0.0053853	Paxs	211.55	Joback Method
dvisc	0.0027288	Paxs	242.73	Joback Method
dvisc	0.0016142	Paxs	273.90	Joback Method
dvisc	0.0010630	Paxs	305.08	Joback Method
dvisc	0.0007564	Paxs	336.26	Joback Method
dvisc	0.0005702	Paxs	367.43	Joback Method
dvisc	0.0004493	Paxs	398.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	330.20	K	1.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C6940767&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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