Methane, triiodo-

Other names:	CARBON TRIIODIDE
	CHI3
	IODOFORM
	Jodoform
	NCI-C04568
	Triiodomethane
	Trijodmethane
Inchi:	InChI=1S/CHI3/c2-1(3)4/h1H
InchiKey:	OKJPEAGHQZHRQV-UHFFFAOYSA-N
Formula:	CHI3
SMILES:	IC(I)I
Mol. weight [g/mol]:	393.73
CAS:	75-47-8

Physical Properties

Property code	Value	Unit	Source
af	0.1930		KDB
chs	-717.50 ± 0.60	kJ/mol	NIST Webbook
gf	129.46	kJ/mol	Joback Method
hf	161.36	kJ/mol	Joback Method
hfs	181.10 ± 1.00	kJ/mol	NIST Webbook
hfus	8.04	kJ/mol	Joback Method
hvap	45.55	kJ/mol	Joback Method
ie	9.25 ± 0.02	eV	NIST Webbook
ie	9.23 ± 0.02	eV	NIST Webbook
ie	9.21	eV	NIST Webbook
log10ws	-4.19		Crippen Method
logp	2.575		Crippen Method
mcvol	102.410	ml/mol	McGowan Method
pc	5310.00	kPa	KDB
rinpol	1221.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1173.00		NIST Webbook
tb	491.20	K	KDB
tc	794.60	K	KDB
tf	392.15 ± 1.50	K	NIST Webbook
tf	398.00 ± 0.60	K	NIST Webbook

tf	391.25 ± 0.50	K	NIST Webbook
tf	394.25 ± 0.40	K	NIST Webbook
tf	392.00 ± 2.00	K	NIST Webbook
tf	396.00	K	KDB
vc	0.349	m3/kmol	KDB
zc	0.2809030		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.75	J/mol×K	501.26	Joback Method
cpg	93.23	J/mol×K	552.87	Joback Method
cpg	94.29	J/mol×K	604.47	Joback Method
cpg	95.02	J/mol×K	656.08	Joback Method
cpg	95.53	J/mol×K	707.68	Joback Method
cpg	95.92	J/mol×K	759.29	Joback Method
cpg	96.28	J/mol×K	810.89	Joback Method
cps	157.50	J/mol×K	298.15	NIST Webbook
dvisc	0.0073475	Pa×s	260.21	Joback Method
dvisc	0.0033835	Pa×s	300.38	Joback Method
dvisc	0.0018709	Pa×s	340.56	Joback Method
dvisc	0.0011723	Pa×s	380.74	Joback Method
dvisc	0.0008031	Pa×s	420.91	Joback Method
dvisc	0.0005877	Pa×s	461.09	Joback Method
dvisc	0.0004521	Pa×s	501.26	Joback Method
hsubt	69.90	kJ/mol	336.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29169e+01
Coeff. B	-2.23182e+03
Coeff. C	-2.14211e+02
Temperature range (K), min.	390.93
Temperature range (K), max.	518.96

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.15223e+01
Coeff. B	-4.73904e+03
Coeff. C	4.32434e-01
Coeff. D	2.28188e-07
Temperature range (K), min.	410.15
Temperature range (K), max.	794.55

Sources

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=1522
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/mol1522.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75478&Units=SI

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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