Benzene, 1-iodo-3-methyl-

Other names:	1-Iodo-3-methylbenzene
	3-Iodotoluene
	Toluene, m-iodo-
	m-Iodotoluene
	m-Methyliodobenzene
Inchi:	InChI=1S/C7H7I/c1-6-3-2-4-7(8)5-6/h2-5H,1H3
InchiKey:	VLCPISYURGTGLP-UHFFFAOYSA-N
Formula:	C7H7I
SMILES:	Cc1cccc(I)c1
Mol. weight [g/mol]:	218.03
CAS:	625-95-6

Physical Properties

Property code	Value	Unit	Source
chl	-3834.20 ± 4.20	kJ/mol	NIST Webbook
gf	168.96	kJ/mol	Joback Method
hf	133.00 ± 5.90	kJ/mol	NIST Webbook
hfl	79.10 ± 4.20	kJ/mol	NIST Webbook
hfus	11.94	kJ/mol	Joback Method
hvap	54.40 ± 4.20	kJ/mol	NIST Webbook
ie	8.60 ± 0.10	eV	NIST Webbook
ie	8.61 ± 0.03	eV	NIST Webbook
log10ws	-3.10		Crippen Method
logp	2.600		Crippen Method
mcvol	111.550	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1121.80		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1121.80		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1148.00		NIST Webbook
ripol	1674.00		NIST Webbook
tb	486.20	K	NIST Webbook
tc	737.63	K	Joback Method
tf	265.65	K	Joback Method

vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.77	J/mol×K	484.36	Joback Method
cpg	193.27	J/mol×K	526.57	Joback Method
cpg	202.97	J/mol×K	568.78	Joback Method
cpg	211.92	J/mol×K	610.99	Joback Method
cpg	220.18	J/mol×K	653.20	Joback Method
cpg	227.78	J/mol×K	695.42	Joback Method
cpg	234.79	J/mol×K	737.63	Joback Method
dvisc	0.0029563	Pa×s	265.65	Joback Method
dvisc	0.0016327	Pa×s	302.10	Joback Method
dvisc	0.0010247	Pa×s	338.55	Joback Method
dvisc	0.0007040	Pa×s	375.00	Joback Method
dvisc	0.0005170	Pa×s	411.46	Joback Method
dvisc	0.0003992	Pa×s	447.91	Joback Method
dvisc	0.0003205	Pa×s	484.36	Joback Method
pvap	7.15e-03	kPa	275.70	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	9.36e-03	kPa	279.30	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.01	kPa	283.50	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.02	kPa	286.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.01	kPa	281.90	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.02	kPa	289.30	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.02	kPa	289.30	Thermochemistry of Halogen-Substituted Methylbenzenes

pvap	0.03	kPa	293.10	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.03	kPa	293.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.04	kPa	298.10	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.04	kPa	298.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.08	kPa	308.00	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.08	kPa	308.00	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.05	kPa	302.90	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.06	kPa	302.90	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.11	kPa	313.10	Thermochemistry of Halogen-Substituted Methylbenzenes

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.20	K	1.30	NIST Webbook

Correlations

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

Coeff. A	1.39134e+01
Coeff. B	-3.81005e+03
Coeff. C	-7.63000e+01
Temperature range (K), min.	355.92
Temperature range (K), max.	519.23

Sources

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
Thermochemistry of Halogen-Substituted Methylbenzenes:	https://www.doi.org/10.1021/je500784s
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=C625956&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume