Benzene, 1-iodo-4-methyl-

Other names:	1-Iodo-4-methylbenzene
	1-Methyl-4-iodobenzene
	4-Iodotoluene
	Toluene, p-iodo-
	p-Iodotoluene
	p-Methyliodobenzene
	p-Tolyl iodide
	toluene, 4-iodo-
Inchi:	InChI=1S/C7H7I/c1-6-2-4-7(8)5-3-6/h2-5H,1H3
InchiKey:	UDHAWRUAECEBHC-UHFFFAOYSA-N
Formula:	C7H7I
SMILES:	Cc1ccc(I)cc1
Mol. weight [g/mol]:	218.03
CAS:	624-31-7

Physical Properties

Property code	Value	Unit	Source
chl	-3822.50 ± 4.20	kJ/mol	NIST Webbook
gf	168.96	kJ/mol	Joback Method
hf	122.00 ± 5.90	kJ/mol	NIST Webbook
hfl	67.40 ± 4.20	kJ/mol	NIST Webbook
hfus	11.94	kJ/mol	Joback Method
hvap	54.40 ± 4.20	kJ/mol	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.38	eV	NIST Webbook
ie	8.60 ± 0.10	eV	NIST Webbook
ie	8.08	eV	NIST Webbook
ie	8.50 ± 0.01	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
ripol	1668.00		NIST Webbook
tb	486.00 ± 2.00	K	NIST Webbook
tb	484.70	K	NIST Webbook
tb	487.65 ± 0.60	K	NIST Webbook
tb	487.65 ± 0.40	K	NIST Webbook

tc	737.63	K	Joback Method
tf	307.50	K	Thermochemistry of Halogen-Substituted Methylbenzenes
tf	308.15 ± 0.60	K	NIST Webbook
tf	310.00 ± 1.00	K	NIST Webbook
tf	307.15 ± 1.50	K	NIST Webbook
tf	307.00 ± 1.50	K	NIST Webbook
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.78	J/mol×K	695.42	Joback Method
cpg	220.18	J/mol×K	653.20	Joback Method
cpg	211.92	J/mol×K	610.99	Joback Method
cpg	202.97	J/mol×K	568.78	Joback Method
cpg	193.27	J/mol×K	526.57	Joback Method
cpg	182.77	J/mol×K	484.36	Joback Method
cpg	234.79	J/mol×K	737.63	Joback Method
dvisc	0.0029563	Pa×s	265.65	Joback Method
dvisc	0.0003205	Pa×s	484.36	Joback Method
dvisc	0.0003992	Pa×s	447.91	Joback Method
dvisc	0.0005170	Pa×s	411.46	Joback Method
dvisc	0.0007040	Pa×s	375.00	Joback Method
dvisc	0.0010247	Pa×s	338.55	Joback Method
dvisc	0.0016327	Pa×s	302.10	Joback Method
hfust	14.96	kJ/mol	306.70	NIST Webbook
hfust	14.96	kJ/mol	306.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38716e+01
Coeff. B	-3.78418e+03
Coeff. C	-7.57440e+01
Temperature range (K), min.	354.32

Temperature range (K), max.	517.81

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624317&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
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

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
hfust:	Enthalpy of fusion 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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