Benzene, (iodomethyl)-

Other names:	(Iodomethyl)benzene
	Benzyl iodide
	Fraissite
	Iodophenylmethane
	Toluene, «alpha»-iodo-
	Toluene, Â«alphaÂ»-iodo-
	UN 2653
	«alpha»-Iodotoluene
	Â«alphaÂ»-Iodotoluene
Inchi:	InChI=1S/C7H7I/c8-6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	XJTQJERLRPWUGL-UHFFFAOYSA-N
Formula:	C7H7I
SMILES:	ICc1ccccc1
Mol. weight [g/mol]:	218.03
CAS:	620-05-3

Physical Properties

Property code	Value	Unit	Source
gf	178.59	kJ/mol	Joback Method
hf	127.30 ± 1.30	kJ/mol	NIST Webbook
hfl	53.00 ± 2.00	kJ/mol	NIST Webbook
hfus	12.33	kJ/mol	Joback Method
hvap	57.70	kJ/mol	NIST Webbook
hvap	57.40 ± 0.30	kJ/mol	NIST Webbook
hvap	50.60 ± 1.40	kJ/mol	NIST Webbook
ie	8.73 ± 0.02	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.91	eV	NIST Webbook
log10ws	-3.30		Crippen Method
logp	2.622		Crippen Method
mcvol	111.550	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
rinpol	1174.00		NIST Webbook
tb	479.38	K	Joback Method
tc	731.20	K	Joback Method
tf	299.45 ± 0.50	K	NIST Webbook
tf	297.60	K	NIST Webbook

vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.02	J/mol×K	479.38	Joback Method
cpg	194.03	J/mol×K	521.35	Joback Method
cpg	204.14	J/mol×K	563.32	Joback Method
cpg	213.42	J/mol×K	605.29	Joback Method
cpg	221.92	J/mol×K	647.26	Joback Method
cpg	229.71	J/mol×K	689.23	Joback Method
cpg	236.84	J/mol×K	731.20	Joback Method
dvisc	0.0020961	Pa×s	290.84	Joback Method
dvisc	0.0042031	Pa×s	253.13	Joback Method
dvisc	0.0012263	Pa×s	328.55	Joback Method
dvisc	0.0008012	Pa×s	366.25	Joback Method
dvisc	0.0005667	Pa×s	403.96	Joback Method
dvisc	0.0004253	Pa×s	441.67	Joback Method
dvisc	0.0003339	Pa×s	479.38	Joback Method
hfust	13.20	kJ/mol	299.50	NIST Webbook
hfust	13.20	kJ/mol	299.50	NIST Webbook
hvapt	46.80	kJ/mol	380.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.20	K	1.30	NIST Webbook
tbrp	366.00	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38427e+01

Coeff. B	-3.78202e+03
Coeff. C	-7.59750e+01
Temperature range (K), min.	354.99
Temperature range (K), max.	519.29

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620053&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume