Benzene, (1-iodoethyl)-

Other names:	1-iodo-1-phenylethane
	(1-Iodoethyl)benzene
Inchi:	InChI=1S/C8H9I/c1-7(9)8-5-3-2-4-6-8/h2-7H,1H3
InchiKey:	HOVGFTKZAOQJEF-UHFFFAOYSA-N
Formula:	C8H9I
SMILES:	CC(I)c1ccccc1
Mol. weight [g/mol]:	232.06
CAS:	10604-60-1

Physical Properties

Property code	Value	Unit	Source
gf	184.57	kJ/mol	Joback Method
hf	99.67	kJ/mol	Joback Method
hfus	11.40	kJ/mol	Joback Method
hvap	59.90 ± 0.40	kJ/mol	NIST Webbook
log10ws	-3.68		Crippen Method
logp	3.183		Crippen Method
mcvol	125.640	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
rinpol	1222.00		NIST Webbook
rinpol	1222.00		NIST Webbook
tb	501.82	K	Joback Method
tc	754.86	K	Joback Method
tf	249.40	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.01	J/mol×K	501.82	Joback Method
cpg	277.98	J/mol×K	712.69	Joback Method
cpg	268.94	J/mol×K	670.51	Joback Method
cpg	259.09	J/mol×K	628.34	Joback Method
cpg	248.36	J/mol×K	586.17	Joback Method

cpg	236.69	J/mol×K	543.99	Joback Method
cpg	286.27	J/mol×K	754.86	Joback Method
dvisc	0.0002919	Pa×s	501.82	Joback Method
dvisc	0.0003831	Pa×s	459.75	Joback Method
dvisc	0.0005310	Pa×s	417.68	Joback Method
dvisc	0.0007919	Pa×s	375.61	Joback Method
dvisc	0.0013062	Pa×s	333.54	Joback Method
dvisc	0.0024895	Pa×s	291.47	Joback Method
dvisc	0.0058981	Pa×s	249.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10604601&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume