

Benzene, 1-ethyl-4-iodo-

Inchi:	InChI=1S/C8H9I/c1-2-7-3-5-8(9)6-4-7/h3-6H,2H2,1H3
InchiKey:	OOLSRHZMXAYDFB-UHFFFAOYSA-N
Formula:	C8H9I
SMILES:	CCc1ccc(I)cc1
Mol. weight [g/mol]:	232.06
CAS:	25309-64-2

Physical Properties

Property code	Value	Unit	Source
gf	177.38	kJ/mol	Joback Method
hf	93.48	kJ/mol	Joback Method
hfus	14.53	kJ/mol	Joback Method
hvap	45.71	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.854		Crippen Method
mcvol	125.640	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
tb	507.24	K	Joback Method
tc	755.48	K	Joback Method
tf	276.92	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.40	J/mol×K	507.24	Joback Method
cpg	235.23	J/mol×K	548.61	Joback Method
cpg	246.21	J/mol×K	589.99	Joback Method
cpg	256.37	J/mol×K	631.36	Joback Method
cpg	265.78	J/mol×K	672.73	Joback Method
cpg	274.48	J/mol×K	714.10	Joback Method
cpg	282.53	J/mol×K	755.48	Joback Method
dvisc	0.0029656	Pa×s	276.92	Joback Method
dvisc	0.0016016	Pa×s	315.31	Joback Method

dvisc	0.0009887	Pa×s	353.69	Joback Method
dvisc	0.0006708	Pa×s	392.08	Joback Method
dvisc	0.0004878	Pa×s	430.47	Joback Method
dvisc	0.0003736	Pa×s	468.85	Joback Method
dvisc	0.0002980	Pa×s	507.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25309642&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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