

Benzene, 1-ethyl-2-iodo-

Other names:	1-ethyl-2-iodobenzene
Inchi:	InChI=1S/C8H9I/c1-2-7-5-3-4-6-8(7)9/h3-6H,2H2,1H3
InchiKey:	ZEJZDNMOGNIHL-UHFFFAOYSA-N
Formula:	C8H9I
SMILES:	CCc1ccccc1I
Mol. weight [g/mol]:	232.06
CAS:	18282-40-1

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.40	J/molxK	507.24	Joback Method
cpg	274.48	J/molxK	714.10	Joback Method
cpg	265.78	J/molxK	672.73	Joback Method
cpg	256.37	J/molxK	631.36	Joback Method
cpg	246.21	J/molxK	589.99	Joback Method
cpg	235.23	J/molxK	548.61	Joback Method
cpg	282.53	J/molxK	755.48	Joback Method
dvisc	0.0002980	Paxs	507.24	Joback Method

dvisc	0.0003736	Paxs	468.85	Joback Method
dvisc	0.0004878	Paxs	430.47	Joback Method
dvisc	0.0006708	Paxs	392.08	Joback Method
dvisc	0.0009887	Paxs	353.69	Joback Method
dvisc	0.0016016	Paxs	315.31	Joback Method
dvisc	0.0029656	Paxs	276.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18282401&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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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