Ethanone, 2-iodo-1-phenyl-

Inchi: InChI=1S/C8H7IO/c9-6-8(10)7-4-2-1-3-5-7/h1-5H,6H2
InchiKey: CREOHKRPSSUXCW-UHFFFAOYSA-N
Formula: C8H7IO
SMILES: O=C(CI)c1ccccc1
Mol. weight [g/mol]: 246.05
CAS: 4636-16-2

Physical Properties

Property code	Value	Unit	Source
gf	58.09	kJ/mol	Joback Method
hf	-7.63	kJ/mol	Joback Method
hfus	16.52	kJ/mol	Joback Method
hvap	51.80	kJ/mol	Joback Method
ie	9.21	eV	NIST Webbook
log10ws	-3.08		Crippen Method
logp	2.304		Crippen Method
mcvol	127.210	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
tb	556.13	K	Joback Method
tc	812.26	K	Joback Method
tf	314.33	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.63	J/mol×K	556.13	Joback Method
cpg	281.02	J/mol×K	769.57	Joback Method
cpg	273.52	J/mol×K	726.88	Joback Method
cpg	265.30	J/mol×K	684.19	Joback Method
cpg	256.29	J/mol×K	641.51	Joback Method
cpg	246.43	J/mol×K	598.82	Joback Method
cpg	287.85	J/mol×K	812.26	Joback Method
dvisc	0.0003312	Pa×s	556.13	Joback Method

dvisc	0.0004204	Pa×s	515.83	Joback Method
dvisc	0.0005558	Pa×s	475.53	Joback Method
dvisc	0.0007737	Pa×s	435.23	Joback Method
dvisc	0.0011522	Pa×s	394.93	Joback Method
dvisc	0.0018785	Pa×s	354.63	Joback Method
dvisc	0.0034716	Pa×s	314.33	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4636162&Units=SI

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
ie:	Ionization energy
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