

Ethanone, 1-(3-iodophenyl)-

Inchi:	InChI=1S/C8H7IO/c1-6(10)7-3-2-4-8(9)5-7/h2-5H,1H3
InchiKey:	IWLHOUBDKCKJJQ-UHFFFAOYSA-N
Formula:	C8H7IO
SMILES:	CC(=O)c1cccc(I)c1
Mol. weight [g/mol]:	246.05
CAS:	14452-30-3

Physical Properties

Property code	Value	Unit	Source
gf	48.46	kJ/mol	Joback Method
hf	-19.10	kJ/mol	Joback Method
hfus	16.13	kJ/mol	Joback Method
hvap	52.46	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.494		Crippen Method
mcvol	127.210	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
tb	561.11	K	Joback Method
tc	818.40	K	Joback Method
tf	326.85	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.58	J/mol×K	561.11	Joback Method
cpg	245.01	J/mol×K	603.99	Joback Method
cpg	254.61	J/mol×K	646.87	Joback Method
cpg	263.42	J/mol×K	689.76	Joback Method
cpg	271.49	J/mol×K	732.64	Joback Method
cpg	278.89	J/mol×K	775.52	Joback Method
cpg	285.66	J/mol×K	818.40	Joback Method
dvisc	0.0026506	Paxs	326.85	Joback Method
dvisc	0.0015479	Paxs	365.89	Joback Method

dvisc	0.0010028	Paxs	404.94	Joback Method
dvisc	0.0007012	Paxs	443.98	Joback Method
dvisc	0.0005195	Paxs	483.02	Joback Method
dvisc	0.0004025	Paxs	522.07	Joback Method
dvisc	0.0003232	Paxs	561.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14452303&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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