

# 2-Iodophenol, isoBOC

<b>Inchi:</b>	InChI=1S/C11H13IO3/c1-8(2)7-14-11(13)15-10-6-4-3-5-9(10)12/h3-6,8H,7H2,1-2H3
<b>InchiKey:</b>	SJPLVEATDQGMNA-UHFFFAOYSA-N
<b>Formula:</b>	C11H13IO3
<b>SMILES:</b>	CC(C)COC(=O)Oc1ccccc1I
<b>Mol. weight [g/mol]:</b>	320.12

## Physical Properties

Property code	Value	Unit	Source
gf	-138.72	kJ/mol	Joback Method
hf	-350.74	kJ/mol	Joback Method
hfus	22.76	kJ/mol	Joback Method
hvap	63.57	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.463		Crippen Method
mcvol	181.220	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	674.15	K	Joback Method
tc	912.43	K	Joback Method
tf	390.12	K	Joback Method
vc	0.667	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.27	J/molxK	674.15	Joback Method
cpg	476.49	J/molxK	872.71	Joback Method
cpg	467.04	J/molxK	833.00	Joback Method
cpg	456.72	J/molxK	793.29	Joback Method
cpg	445.49	J/molxK	753.58	Joback Method
cpg	433.35	J/molxK	713.86	Joback Method
cpg	485.07	J/molxK	912.43	Joback Method
dvisc	0.0001321	Paxs	674.15	Joback Method

dvisc	0.0001692	Paxs	626.81	Joback Method
dvisc	0.0002258	Paxs	579.47	Joback Method
dvisc	0.0003170	Paxs	532.13	Joback Method
dvisc	0.0004758	Paxs	484.80	Joback Method
dvisc	0.0007795	Paxs	437.46	Joback Method
dvisc	0.0014397	Paxs	390.12	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R235039&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R235039&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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