

# 5-Chloro-2-iodobenzoic acid

<b>Inchi:</b>	InChI=1S/C7H4ClIO2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,(H,10,11)
<b>InchiKey:</b>	NRPQWTVTBCRPEL-UHFFFAOYSA-N
<b>Formula:</b>	C7H4ClIO2
<b>SMILES:</b>	O=C(O)c1cc(Cl)ccc1I
<b>Mol. weight [g/mol]:</b>	282.46
<b>CAS:</b>	13421-00-6

## Physical Properties

Property code	Value	Unit	Source
gf	-118.34	kJ/mol	Joback Method
hf	-177.90	kJ/mol	Joback Method
hfus	21.44	kJ/mol	Joback Method
hvap	71.96	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.643		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	672.82	K	Joback Method
tc	915.10	K	Joback Method
tf	418.84	K	Joback Method
vc	0.481	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.40	J/molxK	672.82	Joback Method
cpg	249.60	J/molxK	713.20	Joback Method
cpg	255.29	J/molxK	753.58	Joback Method
cpg	260.49	J/molxK	793.96	Joback Method
cpg	265.26	J/molxK	834.34	Joback Method
cpg	269.62	J/molxK	874.72	Joback Method
cpg	273.61	J/molxK	915.10	Joback Method
dvisc	0.0018874	Paxs	418.84	Joback Method
dvisc	0.0008973	Paxs	461.17	Joback Method

dvisc	0.0004834	Paxs	503.50	Joback Method
dvisc	0.0002866	Paxs	545.83	Joback Method
dvisc	0.0001833	Paxs	588.16	Joback Method
dvisc	0.0001244	Paxs	630.49	Joback Method
dvisc	0.0000887	Paxs	672.82	Joback Method

## Sources

<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=C13421006&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13421006&amp;Units=SI</a>
<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>

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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