

# 2-Iodocinnamic acid

<b>Inchi:</b>	InChI=1S/C9H7IO2/c10-8-4-2-1-3-7(8)5-6-9(11)12/h1-6H,(H,11,12)
<b>InchiKey:</b>	SBCFNNJYIXFMFS-UHFFFAOYSA-N
<b>Formula:</b>	C9H7IO2
<b>SMILES:</b>	O=C(O)C=Cc1ccccc1I
<b>Mol. weight [g/mol]:</b>	274.06
<b>CAS:</b>	1643-34-1

## Physical Properties

Property code	Value	Unit	Source
chs	-4081.00	kJ/mol	NIST Webbook
gf	0.28	kJ/mol	Joback Method
hf	-74.75	kJ/mol	Joback Method
hfs	-292.30	kJ/mol	NIST Webbook
hfus	23.01	kJ/mol	Joback Method
hvap	71.32	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.389		Crippen Method
mcvol	142.870	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
tb	680.33	K	Joback Method
tc	918.86	K	Joback Method
tf	393.86	K	Joback Method
vc	0.524	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.82	J/molxK	680.33	Joback Method
cpg	305.06	J/molxK	720.08	Joback Method
cpg	312.63	J/molxK	759.84	Joback Method
cpg	319.62	J/molxK	799.59	Joback Method
cpg	326.08	J/molxK	839.35	Joback Method
cpg	332.10	J/molxK	879.10	Joback Method
cpg	337.74	J/molxK	918.86	Joback Method

dvisc	0.0025799	Paxs	393.86	Joback Method
dvisc	0.0010042	Paxs	441.61	Joback Method
dvisc	0.0004699	Paxs	489.35	Joback Method
dvisc	0.0002516	Paxs	537.10	Joback Method
dvisc	0.0001492	Paxs	584.84	Joback Method
dvisc	0.0000958	Paxs	632.58	Joback Method
dvisc	0.0000654	Paxs	680.33	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=C1643341&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1643341&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>chs:</b>	Standard solid enthalpy of combustion
<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>hfs:</b>	Solid phase 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>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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