

# 2-Iodo-5-methylbenzoic acid

<b>Other names:</b>	Benzoic acid, 2-iodo-5-methyl-
<b>Inchi:</b>	InChI=1S/C8H7IO2/c1-5-2-3-7(9)6(4-5)8(10)11/h2-4H,1H3,(H,10,11)
<b>InchiKey:</b>	INGWGCDYAJKXKP-UHFFFAOYSA-N
<b>Formula:</b>	C8H7IO2
<b>SMILES:</b>	<chem>Cc1ccc(I)c(C(=O)O)c1</chem>
<b>Mol. weight [g/mol]:</b>	262.04
<b>CAS:</b>	52548-14-8

## Physical Properties

Property code	Value	Unit	Source
gf	-97.99	kJ/mol	Joback Method
hf	-182.80	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	69.80	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.298		Crippen Method
mcvol	133.080	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	658.27	K	Joback Method
tc	892.83	K	Joback Method
tf	400.19	K	Joback Method
vc	0.488	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.40	J/molxK	658.27	Joback Method
cpg	305.94	J/molxK	853.74	Joback Method
cpg	300.06	J/molxK	814.65	Joback Method
cpg	293.70	J/molxK	775.55	Joback Method
cpg	286.83	J/molxK	736.46	Joback Method
cpg	279.41	J/molxK	697.36	Joback Method
cpg	311.38	J/molxK	892.83	Joback Method
dvisc	0.0000899	Paxs	658.27	Joback Method

dvisc	0.0001279	Paxs	615.26	Joback Method
dvisc	0.0001918	Paxs	572.24	Joback Method
dvisc	0.0003072	Paxs	529.23	Joback Method
dvisc	0.0005347	Paxs	486.22	Joback Method
dvisc	0.0010364	Paxs	443.20	Joback Method
dvisc	0.0023161	Paxs	400.19	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C52548148&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52548148&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>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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