

# 3-Iodo-5-nitrobenzoic acid

<b>Inchi:</b>	InChI=1S/C7H4INO4/c8-5-1-4(7(10)11)2-6(3-5)9(12)13/h1-3H,(H,10,11)
<b>InchiKey:</b>	GFGURBBHVJTXDU-UHFFFAOYSA-N
<b>Formula:</b>	C7H4INO4
<b>SMILES:</b>	O=C(O)c1cc(I)cc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	293.02
<b>CAS:</b>	6313-17-3

## Physical Properties

Property code	Value	Unit	Source
gf	-70.86	kJ/mol	Joback Method
hf	-172.92	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	84.16	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	1.898		Crippen Method
mcvol	136.410	ml/mol	McGowan Method
pc	4795.85	kPa	Joback Method
tb	787.23	K	Joback Method
tc	1045.32	K	Joback Method
tf	532.53	K	Joback Method
vc	0.514	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.45	J/molxK	787.23	Joback Method
cpg	300.44	J/molxK	830.24	Joback Method
cpg	305.86	J/molxK	873.26	Joback Method
cpg	310.74	J/molxK	916.27	Joback Method
cpg	315.16	J/molxK	959.29	Joback Method
cpg	319.15	J/molxK	1002.30	Joback Method
cpg	322.78	J/molxK	1045.32	Joback Method

# Sources

<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=C6313173&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6313173&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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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