

# 2-Iodoanisole

<b>Other names:</b>	1-iodo-2-methoxybenzene Anisole, o-iodo- Benzene, 1-iodo-2-methoxy- Iodanisol o-Anisyl iodide o-Iodoanisole
<b>Inchi:</b>	InChI=1S/C7H7IO/c1-9-7-5-3-2-4-6(7)8/h2-5H,1H3
<b>InchiKey:</b>	DVQWNQBEUKXONL-UHFFFAOYSA-N
<b>Formula:</b>	C7H7IO
<b>SMILES:</b>	COc1ccccc1I
<b>Mol. weight [g/mol]:</b>	234.03
<b>CAS:</b>	529-28-2

## Physical Properties

Property code	Value	Unit	Source
gf	63.96	kJ/mol	Joback Method
hf	-18.10	kJ/mol	Joback Method
hfus	13.13	kJ/mol	Joback Method
hvap	45.90	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.300		Crippen Method
mcvol	117.420	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
rinpola	1268.40		NIST Webbook
tb	506.78	K	Joback Method
tc	756.60	K	Joback Method
tf	287.88	K	Joback Method
vc	0.425	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.25	J/mol×K	756.60	Joback Method
cpg	248.13	J/mol×K	714.96	Joback Method

cpg	240.42	J/molxK	673.33	Joback Method
cpg	232.11	J/molxK	631.69	Joback Method
cpg	223.17	J/molxK	590.05	Joback Method
cpg	213.57	J/molxK	548.42	Joback Method
cpg	203.29	J/molxK	506.78	Joback Method
dvisc	0.0022544	Paxs	287.88	Joback Method
dvisc	0.0002641	Paxs	506.78	Joback Method
dvisc	0.0003286	Paxs	470.30	Joback Method
dvisc	0.0004244	Paxs	433.81	Joback Method
dvisc	0.0005743	Paxs	397.33	Joback Method
dvisc	0.0008261	Paxs	360.85	Joback Method
dvisc	0.0012898	Paxs	324.36	Joback Method
hvapt	65.30	kJ/mol	298.15	Experimental and computational study of the molecular energetics of the monoiodoanisole isomers

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.70	K	2.50	NIST Webbook
tbrp	512.70	K	97.30	NIST Webbook

## 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=C529282&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C529282&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>
<b>Experimental and computational study of the molecular energetics of the monoiodoanisole isomers:</b>	<a href="https://www.doi.org/10.1016/j.jct.2011.12.001">https://www.doi.org/10.1016/j.jct.2011.12.001</a>

## Legend

**cpg:** 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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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