

# Isochavicol

<b>Inchi:</b>	InChI=1S/C9H10O/c1-2-3-8-4-6-9(10)7-5-8/h2-7,10H,1H3/b3-2+
<b>InchiKey:</b>	UMFCIIBZHQXRCJ-NSCUHMNNSA-N
<b>Formula:</b>	C9H10O
<b>SMILES:</b>	CC=Cc1ccc(O)cc1
<b>Mol. weight [g/mol]:</b>	134.18

## Physical Properties

Property code	Value	Unit	Source
gf	62.91	kJ/mol	Joback Method
hf	-52.65	kJ/mol	Joback Method
hfus	19.09	kJ/mol	Joback Method
hvap	50.88	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.425		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	1313.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1313.00		NIST Webbook
tb	516.78	K	Joback Method
tc	749.81	K	Joback Method
tf	324.25	K	Joback Method
vc	0.378	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.07	J/molxK	516.78	Joback Method
cpg	261.39	J/molxK	555.62	Joback Method
cpg	272.71	J/molxK	594.46	Joback Method
cpg	283.12	J/molxK	633.30	Joback Method
cpg	292.74	J/molxK	672.13	Joback Method
cpg	301.67	J/molxK	710.97	Joback Method

cpg	310.01	J/molxK	749.81	Joback Method
dvisc	0.0042810	Paxs	324.25	Joback Method
dvisc	0.0015405	Paxs	356.34	Joback Method
dvisc	0.0006563	Paxs	388.43	Joback Method
dvisc	0.0003185	Paxs	420.51	Joback Method
dvisc	0.0001713	Paxs	452.60	Joback Method
dvisc	0.0001000	Paxs	484.69	Joback Method
dvisc	0.0000624	Paxs	516.78	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R614254&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R614254&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>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>

## 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>rinpol:</b>	Non-polar retention indices
<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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