

# Isonopinone

<b>Inchi:</b>	InChI=1S/C9H14O/c1-9(2)6-3-7(9)5-8(10)4-6/h6-7H,3-5H2,1-2H3
<b>InchiKey:</b>	YMCXBJXUNDYDTO-UHFFFAOYSA-N
<b>Formula:</b>	C9H14O
<b>SMILES:</b>	CC1(C)C2CC(=O)CC1C2
<b>Mol. weight [g/mol]:</b>	138.21

## Physical Properties

Property code	Value	Unit	Source
gf	-1.49	kJ/mol	Joback Method
hf	-232.45	kJ/mol	Joback Method
hfus	7.52	kJ/mol	Joback Method
hvap	38.41	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	2.012		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
rinpol	1088.00		NIST Webbook
ripol	1496.00		NIST Webbook
tb	486.46	K	Joback Method
tc	713.39	K	Joback Method
tf	311.43	K	Joback Method
vc	0.450	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.51	J/molxK	486.46	Joback Method
cpg	296.15	J/molxK	524.28	Joback Method
cpg	312.56	J/molxK	562.10	Joback Method
cpg	327.88	J/molxK	599.93	Joback Method
cpg	342.24	J/molxK	637.75	Joback Method
cpg	355.78	J/molxK	675.57	Joback Method
cpg	368.63	J/molxK	713.39	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=R512935&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R512935&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	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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