

# 2-Hydroxyisodavanone D

<b>Inchi:</b>	InChI=1S/C15H24O3/c1-6-15(5)10-8-13(18-15)11(2)12(16)7-9-14(3,4)17/h6-7,9,11,13,17
<b>InchiKey:</b>	WQUKMIHCFQFPQG-PXBZKYGSSA-N
<b>Formula:</b>	C15H24O3
<b>SMILES:</b>	<chem>C=CC1(C)CCC(C(C)C(=O)C=CC(C)(C)O)O1</chem>
<b>Mol. weight [g/mol]:</b>	252.35

## Physical Properties

Property code	Value	Unit	Source
gf	-84.63	kJ/mol	Joback Method
hf	-465.74	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.642		Crippen Method
mcvol	216.060	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinqol	1652.00		NIST Webbook
tb	723.62	K	Joback Method
tc	929.03	K	Joback Method
tf	407.27	K	Joback Method
vc	0.803	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.58	J/mol×K	723.62	Joback Method
cpg	657.78	J/mol×K	757.86	Joback Method
cpg	673.27	J/mol×K	792.09	Joback Method
cpg	688.20	J/mol×K	826.33	Joback Method
cpg	702.71	J/mol×K	860.56	Joback Method
cpg	716.96	J/mol×K	894.80	Joback Method
cpg	731.08	J/mol×K	929.03	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=R226634&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R226634&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>

# 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>hvac:</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>mccvol:</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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