

# Isoacorone

<b>Other names:</b>	[1R-(1«alpha»,4«beta»,5«beta»,8S*)]-1-isopropyl-4,8-dimethylspiro[4.5]decane-2,7-dione
<b>Inchi:</b>	InChI=1S/C15H24O2/c1-9(2)14-12(16)7-11(4)15(14)6-5-10(3)13(17)8-15/h9-11,14H,5-8H
<b>InchiKey:</b>	AGUISGUERLMHFF-RBDSIQFVSA-N
<b>Formula:</b>	C15H24O2
<b>SMILES:</b>	CC1CCC2(CC1=O)C(C)CC(=O)C2C(C)C
<b>Mol. weight [g/mol]:</b>	236.35
<b>CAS:</b>	6168-64-5

## Physical Properties

Property code	Value	Unit	Source
gf	-120.01	kJ/mol	Joback Method
hf	-538.09	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	55.83	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.243		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1771.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	699.26	K	Joback Method
tc	941.42	K	Joback Method
tf	417.47	K	Joback Method
vc	0.761	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.74	J/molxK	699.26	Joback Method
cpg	652.57	J/molxK	739.62	Joback Method
cpg	675.10	J/molxK	779.98	Joback Method

cpg	696.41	J/mol×K	820.34	Joback Method
cpg	716.60	J/mol×K	860.70	Joback Method
cpg	735.80	J/mol×K	901.06	Joback Method
cpg	754.08	J/mol×K	941.42	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6168645&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6168645&amp;Units=SI</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>rinpola:</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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