

# (3S,6S)-6-Isopropyl-3-methyl-2-(propan-2-ylidene)

<b>Inchi:</b>	InChI=1S/C15H24O/c1-7-15(6)9-8-12(10(2)3)14(16)13(15)11(4)5/h7,10,12H,1,8-9H2,2-6
<b>InchiKey:</b>	YMIHAYABXZORPU-DOMZBBRYSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	<chem>C=CC1(C)CCC(C(C)C)C(=O)C1=C(C)C</chem>
<b>Mol. weight [g/mol]:</b>	220.35
<b>CAS:</b>	21698-46-4

## Physical Properties

Property code	Value	Unit	Source
gf	86.39	kJ/mol	Joback Method
hf	-255.02	kJ/mol	Joback Method
hfus	14.93	kJ/mol	Joback Method
hvap	52.01	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	4.150		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1854.71	kPa	Joback Method
tb	628.30	K	Joback Method
tc	851.27	K	Joback Method
tf	333.71	K	Joback Method
vc	0.771	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.73	J/molxK	628.30	Joback Method
cpg	574.02	J/molxK	665.46	Joback Method
cpg	594.20	J/molxK	702.62	Joback Method
cpg	613.39	J/molxK	739.79	Joback Method
cpg	631.70	J/molxK	776.95	Joback Method
cpg	649.23	J/molxK	814.11	Joback Method
cpg	666.10	J/molxK	851.27	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=C21698464&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21698464&amp;Units=SI</a>
<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>

# 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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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