

# «beta»-Selinen-2«alpha»-ol (Jatamol A)

<b>Inchi:</b>	InChI=1S/C15H24O/c1-10(2)12-8-13-11(3)6-5-7-15(13,4)14(16)9-12/h12-14,16H,1,3,5-9
<b>InchiKey:</b>	BFMDGLARCCRDW-LRMYVUMKSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	C=C(C)C1CC(O)C2(C)CCCC(=C)C2C1
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	123.16	kJ/mol	Joback Method
hf	-209.76	kJ/mol	Joback Method
hfus	18.66	kJ/mol	Joback Method
hvap	63.98	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinsol	1690.00		NIST Webbook
tb	651.96	K	Joback Method
tc	859.17	K	Joback Method
tf	354.81	K	Joback Method
vc	0.739	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.06	J/mol×K	651.96	Joback Method
cpg	592.62	J/mol×K	686.50	Joback Method
cpg	611.16	J/mol×K	721.03	Joback Method
cpg	628.80	J/mol×K	755.57	Joback Method
cpg	645.67	J/mol×K	790.10	Joback Method
cpg	661.88	J/mol×K	824.64	Joback Method
cpg	677.55	J/mol×K	859.17	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=R232901&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R232901&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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