

# (11E,13Z)-Labdadien-8-ol

<b>Inchi:</b>	InChI=1S/C20H34O/c1-7-15(2)9-10-17-19(5)13-8-12-18(3,4)16(19)11-14-20(17,6)21/h7,9,11,13,15,17,19,21
<b>InchiKey:</b>	FUOYNUQYIXMTMU-KHYUXNBXSA-N
<b>Formula:</b>	C20H34O
<b>SMILES:</b>	CC=C(C)C=CC1C(C)(O)CCC2C(C)(C)CCCC21C
<b>Mol. weight [g/mol]:</b>	290.48

## Physical Properties

Property code	Value	Unit	Source
gf	166.09	kJ/mol	Joback Method
hf	-278.05	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	72.92	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.502		Crippen Method
mcvol	268.210	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinsol	2095.00		NIST Webbook
tb	774.65	K	Joback Method
tc	990.52	K	Joback Method
tf	432.64	K	Joback Method
vc	1.008	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.84	J/mol×K	774.65	Joback Method
cpg	882.67	J/mol×K	810.63	Joback Method
cpg	906.55	J/mol×K	846.61	Joback Method
cpg	930.82	J/mol×K	882.59	Joback Method
cpg	955.83	J/mol×K	918.57	Joback Method
cpg	981.92	J/mol×K	954.54	Joback Method
cpg	1009.42	J/mol×K	990.52	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=R202103&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202103&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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