

# Linalool oxide isomer # 2

<b>Inchi:</b>	InChI=1S/C10H18O2/c1-5-10(4)7-6-8(12-10)9(2,3)11/h5,8,11H,1,6-7H2,2-4H3
<b>InchiKey:</b>	BRHDDEIRQPDPMG-UHFFFAOYSA-N
<b>Formula:</b>	C10H18O2
<b>SMILES:</b>	C=CC1(C)CCC(C(C)(C)O)O1
<b>Mol. weight [g/mol]:</b>	170.25

## Physical Properties

Property code	Value	Unit	Source
gf	-75.59	kJ/mol	Joback Method
hf	-361.90	kJ/mol	Joback Method
hfus	13.74	kJ/mol	Joback Method
hvap	55.87	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.881		Crippen Method
mvol	148.340	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
ripol	1472.00		NIST Webbook
ripol	1472.00		NIST Webbook
tb	551.63	K	Joback Method
tc	752.27	K	Joback Method
tf	321.07	K	Joback Method
vc	0.543	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.75	J/mol×K	551.63	Joback Method
cpg	399.17	J/mol×K	585.07	Joback Method
cpg	413.59	J/mol×K	618.51	Joback Method
cpg	427.13	J/mol×K	651.95	Joback Method
cpg	439.91	J/mol×K	685.39	Joback Method
cpg	452.03	J/mol×K	718.83	Joback Method
cpg	463.60	J/mol×K	752.27	Joback Method

# Sources

<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=R610425&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R610425&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>ri pol:</b>	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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