

# Linalool oxide II (pyran)

<b>Other names:</b>	linalool oxide D (cis-THP) Linalool oxide II (pyranoid) linalool oxide (IV)
<b>Inchi:</b>	InChI=1S/C10H18O2/c1-5-10(4)7-6-8(11)9(2,3)12-10/h5,8,11H,1,6-7H2,2-4H3
<b>InchiKey:</b>	BCTBAGTXFYWYMW-UHFFFAOYSA-N
<b>Formula:</b>	C10H18O2
<b>SMILES:</b>	C=CC1(C)CCC(O)C(C)(C)O1
<b>Mol. weight [g/mol]:</b>	170.25

## Physical Properties

Property code	Value	Unit	Source
gf	-103.73	kJ/mol	Joback Method
hf	-364.41	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	55.88	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.881		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpole	1145.00		NIST Webbook
rinpole	1174.00		NIST Webbook
ripole	1769.00		NIST Webbook
ripole	1776.00		NIST Webbook
ripole	1772.00		NIST Webbook
ripole	1721.00		NIST Webbook
tb	554.70	K	Joback Method
tc	757.96	K	Joback Method
tf	334.79	K	Joback Method
vc	0.543	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.60	J/molxK	554.70	Joback Method

cpg	397.07	J/mol×K	588.58	Joback Method
cpg	411.62	J/mol×K	622.45	Joback Method
cpg	425.40	J/mol×K	656.33	Joback Method
cpg	438.57	J/mol×K	690.21	Joback Method
cpg	451.29	J/mol×K	724.08	Joback Method
cpg	463.72	J/mol×K	757.96	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=R196137&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R196137&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>rinpol:</b>	Non-polar retention indices
<b>ripol:</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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