

# Lilac alcohol (isomer IV)

<b>Inchi:</b>	InChI=1S/C10H18O2/c1-4-10(3)6-5-9(12-10)8(2)7-11/h4,8-9,11H,1,5-7H2,2-3H3
<b>InchiKey:</b>	VUEGXHXUMOKKN-UHFFFAOYSA-N
<b>Formula:</b>	C10H18O2
<b>SMILES:</b>	C=CC1(C)CCC(C(C)CO)O1
<b>Mol. weight [g/mol]:</b>	170.25

## Physical Properties

Property code	Value	Unit	Source
gf	-80.87	kJ/mol	Joback Method
hf	-358.43	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	56.78	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.739		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinsol	1235.00		NIST Webbook
tb	554.42	K	Joback Method
tc	747.74	K	Joback Method
tf	303.65	K	Joback Method
vc	0.548	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.87	J/mol×K	554.42	Joback Method
cpg	395.72	J/mol×K	586.64	Joback Method
cpg	409.73	J/mol×K	618.86	Joback Method
cpg	422.99	J/mol×K	651.08	Joback Method
cpg	435.60	J/mol×K	683.30	Joback Method
cpg	447.63	J/mol×K	715.52	Joback Method
cpg	459.18	J/mol×K	747.74	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=R606689&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R606689&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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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