

# Lilac aldehyde, isomer # 1

<b>Inchi:</b>	InChI=1S/C10H16O2/c1-4-10(3)6-5-9(12-10)8(2)7-11/h4,7-9H,1,5-6H2,2-3H3
<b>InchiKey:</b>	YPZQHCLBLRWNMJ-UHFFFAOYSA-N
<b>Formula:</b>	C10H16O2
<b>SMILES:</b>	C=CC1(C)CCC(C(C)C=O)O1
<b>Mol. weight [g/mol]:</b>	168.23

## Physical Properties

Property code	Value	Unit	Source
gf	-43.57	kJ/mol	Joback Method
hf	-291.78	kJ/mol	Joback Method
hfus	15.83	kJ/mol	Joback Method
hvap	46.82	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	1.945		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
ripol	1550.00		NIST Webbook
tb	510.90	K	Joback Method
tc	721.44	K	Joback Method
tf	284.83	K	Joback Method
vc	0.546	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.23	J/molxK	510.90	Joback Method
cpg	359.67	J/molxK	545.99	Joback Method
cpg	375.04	J/molxK	581.08	Joback Method
cpg	389.45	J/molxK	616.17	Joback Method
cpg	403.00	J/molxK	651.26	Joback Method
cpg	415.80	J/molxK	686.35	Joback Method
cpg	427.97	J/molxK	721.44	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R591270&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R591270&amp;Units=SI</a>
<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>

# 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>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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