

# Lilac aldehyde isomer A

<b>Inchi:</b>	InChI=1S/C11H18O2/c1-5-10(3)6-7-11(4,13-10)9(2)8-12/h5,8-9H,1,6-7H2,2-4H3
<b>InchiKey:</b>	GQKMBIOXFXUQNM-UHFFFAOYSA-N
<b>Formula:</b>	C11H18O2
<b>SMILES:</b>	<chem>C=CC1(C)CCC(C)(C(C)C=O)O1</chem>
<b>Mol. weight [g/mol]:</b>	182.26

## Physical Properties

Property code	Value	Unit	Source
gf	-40.64	kJ/mol	Joback Method
hf	-297.18	kJ/mol	Joback Method
hfus	12.12	kJ/mol	Joback Method
hvap	47.90	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.335		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
tb	534.02	K	Joback Method
tc	749.87	K	Joback Method
tf	320.00	K	Joback Method
vc	0.601	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.71	J/molxK	534.02	Joback Method
cpg	406.62	J/molxK	569.99	Joback Method
cpg	422.33	J/molxK	605.97	Joback Method
cpg	437.04	J/molxK	641.94	Joback Method
cpg	450.97	J/molxK	677.92	Joback Method
cpg	464.31	J/molxK	713.89	Joback Method
cpg	477.27	J/molxK	749.87	Joback Method

# Sources

<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=R417726&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R417726&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>

# 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>rinpola:</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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