Lilac aldehyde A

Other names:	Lilac aldehyde (isomer I) 2-Furanacetaldehyde, 5-ethenyltetrahydro-«alpha»,5-dimethyl-, («alpha»S,2S,5S)- Lilac aldehyde, (2S,2'S,5'S)-
Inchi:	InChI=1S/C10H16O2/c1-4-10(3)6-5-9(12-10)8(2)7-11/h4,7-9H,1,5-6H2,2-3H3
InchiKey:	YPZQHCLBLRWNMJ-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	C=CC1(C)CCC(C(C)C=O)O1
Mol. weight [g/mol]:	168.23
CAS:	53447-46-4

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
rinpol	1145.00		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/mol×K	510.90	Joback Method
cpg	359.67	J/mol×K	545.99	Joback Method
cpg	375.04	J/mol×K	581.08	Joback Method
cpg	389.45	J/mol×K	616.17	Joback Method
cpg	403.00	J/mol×K	651.26	Joback Method

cpg	415.80	J/mol×K	686.35	Joback Method
cpg	427.97	J/mol×K	721.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53447464&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume