Lilac aldehyde, isomer # 3

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

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	1573.00		NIST Webbook
ripol	1573.00		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=R591290&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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