Lilac aldehyde isomer B

Inchi: 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
InchiKey: GQKMBIOXFXUQNM-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: C=CC1(C)CCC(C)(C(C)C=O)O1
Mol. weight [g/mol]: 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	1141.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1141.00		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/mol×K	534.02	Joback Method
cpg	406.62	J/mol×K	569.99	Joback Method
cpg	422.33	J/mol×K	605.97	Joback Method
cpg	437.04	J/mol×K	641.94	Joback Method
cpg	450.97	J/mol×K	677.92	Joback Method
cpg	464.31	J/mol×K	713.89	Joback Method
cpg	477.27	J/mol×K	749.87	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=R417731&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