Lilac alcohol B

Other names:	2-Furanethanol, tetrahydro-«beta»,5-dimethyl-5-vinyl-, («beta»R,2S,5S)-
	Lilac alcohol (isomer II)
Inchi:	InChI=1S/C10H18O2/c1-4-10(3)6-5-9(12-10)8(2)7-11/h4,8-9,11H,1,5-7H2,2-3H3
InchiKey:	VUEGXHXUMOZKKN-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=CC1(C)CCC(C(C)CO)O1
Mol. weight [g/mol]:	170.25
CAS:	33081-35-5

Physical Properties

Property code	Value	Unit	Source
gf	-80.87	kJ/mol	Joback Method
hf	-358.43	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	56.78	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.739		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1212.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1219.00		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1758.00		NIST Webbook
tb	554.42	K	Joback Method
tc	747.74	K	Joback Method
tf	303.65	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	380.87	J/mol×K	554.42	Joback Method
cpg	395.72	J/mol×K	586.64	Joback Method
cpg	409.73	J/mol×K	618.86	Joback Method
cpg	422.99	J/mol×K	651.08	Joback Method
cpg	435.60	J/mol×K	683.30	Joback Method
cpg	447.63	J/mol×K	715.52	Joback Method
cpg	459.18	J/mol×K	747.74	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=C33081355&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume