Lilac alcohol (isomer III)

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

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	1221.00		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:	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=R606674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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