2,7-Octadiene-1,6-diol, 2,6-dimethyl-

Other names:	8-Hydroxylinalool
	2,6-Dimethyl-2,7-octadiene-1,6-diol
	8-Hydroxylinalol
	Hydroxylinalool
	2,6-dimethyl-octadiene-diol (linalool hydroxy)
Inchi:	InChI=1S/C10H18O2/c1-4-10(3,12)7-5-6-9(2)8-11/h4,6,11-12H,1,5,7-8H2,2-3H3/b9-6+
InchiKey:	NSMIMJYEKVSYMT-RMKNXTFCSA-N
Formula:	C10H18O2
SMILES:	C=CC(C)(O)CCC=C(C)CO
Mol. weight [g/mol]:	170.25
CAS:	64142-78-5

Physical Properties

Property code	Value	Unit	Source
gf	-77.97	kJ/mol	Joback Method
hf	-330.08	kJ/mol	Joback Method
hfus	20.03	kJ/mol	Joback Method
hvap	69.28	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.642		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	1336.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1367.40		NIST Webbook
rinpol	1367.40		NIST Webbook
ripol	2251.00		NIST Webbook
ripol	2251.00		NIST Webbook
tb	610.05	K	Joback Method
tc	782.91	K	Joback Method
tf	305.72	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.74	J/mol×K	610.05	Joback Method
cpg	413.76	J/mol×K	638.86	Joback Method
cpg	424.19	J/mol×K	667.67	Joback Method
cpg	434.07	J/mol×K	696.48	Joback Method
cpg	443.45	J/mol×K	725.29	Joback Method
cpg	452.35	J/mol×K	754.10	Joback Method
cpg	460.83	J/mol×K	782.91	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=C64142785&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume