

(E)-8-Hydroxylinalool

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

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
ripol	2265.00		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/molxK	610.05	Joback Method
cpg	413.76	J/molxK	638.86	Joback Method
cpg	424.19	J/molxK	667.67	Joback Method
cpg	434.07	J/molxK	696.48	Joback Method
cpg	443.45	J/molxK	725.29	Joback Method
cpg	452.35	J/molxK	754.10	Joback Method
cpg	460.83	J/molxK	782.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R611126&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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