

5-Hydroxylinalol

Inchi:	InChI=1S/C10H18O2/c1-5-10(4,12)7-9(11)6-8(2)3/h5-6,9,11-12H,1,7H2,2-4H3
InchiKey:	QHPOKHQEHNFX-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=CC(C)(O)CC(O)C=C(C)C
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
gf	-80.41	kJ/mol	Joback Method
hf	-335.36	kJ/mol	Joback Method
hfus	16.51	kJ/mol	Joback Method
hvap	68.90	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.641		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
ripol	2034.00		NIST Webbook
tb	609.61	K	Joback Method
tc	785.25	K	Joback Method
tf	290.72	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.19	J/mol×K	609.61	Joback Method
cpg	414.43	J/mol×K	638.88	Joback Method
cpg	425.05	J/mol×K	668.16	Joback Method
cpg	435.11	J/mol×K	697.43	Joback Method
cpg	444.63	J/mol×K	726.70	Joback Method
cpg	453.67	J/mol×K	755.98	Joback Method
cpg	462.25	J/mol×K	785.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333430&Units=SI
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

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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