hydroxycitronellol

Inchi: InChI=1S/C11H22O2/c1-9(2)7-10(13)8-11(3,4)5-6-12/h7,10,12-13H,5-6,8H2,1-4H3
InchiKey: HVCWFSIXTUOOBZ-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: CC(C)=CC(O)CC(C)(C)CCO
Mol. weight [g/mol]: 186.29

Physical Properties

Property code	Value	Unit	Source
gf	-159.83	kJ/mol	Joback Method
hf	-481.43	kJ/mol	Joback Method
hfus	20.38	kJ/mol	Joback Method
hvap	71.79	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.112		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1329.50		NIST Webbook
tb	635.81	K	Joback Method
tc	808.19	K	Joback Method
tf	303.75	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.34	J/mol×K	635.81	Joback Method
cpg	486.77	J/mol×K	664.54	Joback Method
cpg	498.56	J/mol×K	693.27	Joback Method
cpg	509.77	J/mol×K	722.00	Joback Method
cpg	520.43	J/mol×K	750.73	Joback Method
cpg	530.58	J/mol×K	779.46	Joback Method
cpg	540.25	J/mol×K	808.19	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=R185647&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume