geraniol hydrate

Inchi: InChI=1S/C10H20O2/c1-9(6-8-11)5-4-7-10(2,3)12/h6,11-12H,4-5,7-8H2,1-3H3/b9-6+
InchiKey: JFIQWLBNEDZWHF-RMKNXTFCSA-N
Formula: C10H20O2
SMILES: CC(=CCO)CCCC(C)(C)O
Mol. weight [g/mol]: 172.26

Physical Properties

Property code	Value	Unit	Source
gf	-165.81	kJ/mol	Joback Method
hf	-455.51	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	69.95	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	1.866		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
ripol	2316.00		NIST Webbook
ripol	2344.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2312.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2344.00		NIST Webbook
tb	613.37	K	Joback Method
tc	783.82	K	Joback Method
tf	307.48	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.91	J/mol×K	613.37	Joback Method
cpg	435.51	J/mol×K	641.78	Joback Method
cpg	446.53	J/mol×K	670.19	Joback Method
cpg	457.00	J/mol×K	698.59	Joback Method

cpg	466.95	J/mol×K	727.00	Joback Method
cpg	476.43	J/mol×K	755.41	Joback Method
cpg	485.46	J/mol×K	783.82	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=R302699&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume