geranic acid hydrate

Inchi: InChI=1S/C10H18O3/c1-8(7-9(11)12)5-4-6-10(2,3)13/h7,13H,4-6H2,1-3H3,(H,11,12)/b8-
InchiKey: VRNUANDJOCAWED-BQYQJAHWSA-N
Formula: C10H18O3
SMILES: CC(=CC(=O)O)CCCC(C)(C)O
Mol. weight [g/mol]: 186.25

Physical Properties

Property code	Value	Unit	Source
gf	-294.73	kJ/mol	Joback Method
hf	-568.09	kJ/mol	Joback Method
hfus	22.91	kJ/mol	Joback Method
hvap	76.70	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.958		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
ripol	2836.00		NIST Webbook
tb	667.24	K	Joback Method
tc	845.41	K	Joback Method
tf	357.41	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.73	J/mol×K	667.24	Joback Method
cpg	450.27	J/mol×K	696.93	Joback Method
cpg	460.24	J/mol×K	726.63	Joback Method
cpg	469.69	J/mol×K	756.32	Joback Method
cpg	478.66	J/mol×K	786.02	Joback Method
cpg	487.17	J/mol×K	815.71	Joback Method
cpg	495.27	J/mol×K	845.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333029&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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