Isogeranyl formate

Inchi: InChI=1S/C11H18O2/c1-10(2)5-4-6-11(3)7-8-13-9-12/h5,9H,3-4,6-8H2,1-2H3
InchiKey: OHQYHMHWNJADLT-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: C=C(CCC=C(C)C)CCOC=O
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-11.82	kJ/mol	Joback Method
hf	-265.10	kJ/mol	Joback Method
hfus	24.02	kJ/mol	Joback Method
hvap	48.66	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.852		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1266.00		NIST Webbook
rinpol	1266.00		NIST Webbook
tb	522.76	K	Joback Method
tc	706.04	K	Joback Method
tf	243.20	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.60	J/mol×K	522.76	Joback Method
cpg	392.74	J/mol×K	553.31	Joback Method
cpg	406.22	J/mol×K	583.85	Joback Method
cpg	419.08	J/mol×K	614.40	Joback Method
cpg	431.32	J/mol×K	644.95	Joback Method
cpg	442.98	J/mol×K	675.49	Joback Method
cpg	454.07	J/mol×K	706.04	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=R284110&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

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