Fragranyl acetate

Inchi: InChI=1S/C12H20O2/c1-9(2)11-5-6-12(11,4)7-8-14-10(3)13/h11H,1,5-8H2,2-4H3
InchiKey: HOTBFDJPUVYSFO-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: C=C(C)C1CCC1(C)CCOC(C)=O
Mol. weight [g/mol]: 196.29
CAS: 51117-22-7

Physical Properties

Property code	Value	Unit	Source
gf	-69.02	kJ/mol	Joback Method
hf	-358.63	kJ/mol	Joback Method
hfus	17.84	kJ/mol	Joback Method
hvap	49.50	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.932		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	1345.00		NIST Webbook
tb	553.39	K	Joback Method
tc	754.20	K	Joback Method
tf	315.52	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.45	J/mol×K	553.39	Joback Method
cpg	448.67	J/mol×K	586.86	Joback Method
cpg	464.94	J/mol×K	620.33	Joback Method
cpg	480.35	J/mol×K	653.79	Joback Method
cpg	495.01	J/mol×K	687.26	Joback Method
cpg	508.99	J/mol×K	720.73	Joback Method
cpg	522.41	J/mol×K	754.20	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=C51117227&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