cis-Myrtanyl acetate

Inchi: InChI=1S/C12H20O2/c1-8(13)14-7-9-4-5-10-6-11(9)12(10,2)3/h9-11H,4-7H2,1-3H3/t9-,1
InchiKey: UWHRPSXEBAXLDR-DCAQKATOSA-N
Formula: C12H20O2
SMILES: CC(=O)OCC1CCC2CC1C2(C)C
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-95.27	kJ/mol	Joback Method
hf	-421.81	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	49.69	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.622		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1365.00		NIST Webbook
rinpol	1365.00		NIST Webbook
ripol	1746.00		NIST Webbook
tb	558.90	K	Joback Method
tc	766.28	K	Joback Method
tf	344.94	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.95	J/mol×K	558.90	Joback Method
cpg	457.77	J/mol×K	593.46	Joback Method
cpg	475.48	J/mol×K	628.03	Joback Method
cpg	492.21	J/mol×K	662.59	Joback Method
cpg	508.06	J/mol×K	697.15	Joback Method
cpg	523.16	J/mol×K	731.72	Joback Method
cpg	537.62	J/mol×K	766.28	Joback Method

Sources

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=R512920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume