(-)-4-epi-Marsupellol acetate

Inchi: InChI=1S/C17H26O2/c1-10-13(19-11(2)18)9-12-15-14(10)17(12,5)8-6-7-16(15,3)4/h12-1
InchiKey: RCEFXIVQCAIFDV-ZMBIAZEOSA-N
Formula: C17H26O2
SMILES: C=C1C(OC(C)=O)CC2C3C1C2(C)CCCC3(C)C
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	35.36	kJ/mol	Joback Method
hf	-379.23	kJ/mol	Joback Method
hfus	22.24	kJ/mol	Joback Method
hvap	59.60	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.957		Crippen Method
mcvol	220.950	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook
tb	679.04	K	Joback Method
tc	899.33	K	Joback Method
tf	449.05	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.85	J/mol×K	679.04	Joback Method
cpg	691.60	J/mol×K	715.75	Joback Method
cpg	712.47	J/mol×K	752.47	Joback Method
cpg	732.71	J/mol×K	789.18	Joback Method
cpg	752.57	J/mol×K	825.90	Joback Method
cpg	772.32	J/mol×K	862.61	Joback Method
cpg	792.19	J/mol×K	899.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R302986&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume