4-epi-Marsupellol

Inchi: InChI=1S/C14H22O/c1-8-10(15)7-9-12-11(8)14(9,4)6-5-13(12,2)3/h9-12,15H,1,5-7H2,2-4
InchiKey: BYWVWPAVZNWJQI-CZKGIMFJSA-N
Formula: C14H22O
SMILES: C=C1C(O)CC2C3C1C2(C)CCC3(C)C
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	119.30	kJ/mol	Joback Method
hf	-218.58	kJ/mol	Joback Method
hfus	17.87	kJ/mol	Joback Method
hvap	60.28	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.996		Crippen Method
mcvol	177.110	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1614.00		NIST Webbook
rinpol	1614.00		NIST Webbook
tb	622.02	K	Joback Method
tc	826.45	K	Joback Method
tf	407.42	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.17	J/mol×K	622.02	Joback Method
cpg	537.95	J/mol×K	656.09	Joback Method
cpg	554.83	J/mol×K	690.16	Joback Method
cpg	571.03	J/mol×K	724.23	Joback Method
cpg	586.77	J/mol×K	758.30	Joback Method
cpg	602.26	J/mol×K	792.37	Joback Method
cpg	617.72	J/mol×K	826.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R426116&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