(+)-5-Hydroxymarsupellol acetate

Inchi: InChI=1S/C19H28O4/c1-10-13-14-15(19(13,6)9-7-8-18(14,4)5)17(23-12(3)21)16(10)22-1
InchiKey: SYNMREOKVHJLFP-ZZKWDYDOSA-N
Formula: C19H28O4
SMILES: C=C1C(OC(C)=O)C(OC(C)=O)C2C3C1C2(C)CCCC3(C)C
Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-189.43	kJ/mol	Joback Method
hf	-685.65	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.498		Crippen Method
mcvol	256.570	ml/mol	McGowan Method
pc	1558.58	kPa	Joback Method
rinpol	1856.00		NIST Webbook
rinpol	1856.00		NIST Webbook
tb	796.42	K	Joback Method
tc	1014.11	K	Joback Method
tf	539.51	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.15	J/mol×K	796.42	Joback Method
cpg	866.94	J/mol×K	832.70	Joback Method
cpg	888.41	J/mol×K	868.98	Joback Method
cpg	909.79	J/mol×K	905.27	Joback Method
cpg	931.29	J/mol×K	941.55	Joback Method
cpg	953.13	J/mol×K	977.83	Joback Method
cpg	975.55	J/mol×K	1014.11	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=R302926&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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