5-Hydroxymarsupellyl acetate

Inchi: InChI=1S/C17H26O3/c1-9-11-12-13(14(19)15(9)20-10(2)18)17(11,5)8-6-7-16(12,3)4/h11
InchiKey: SSRSFLZAFQCYHK-ADSVNHKOSA-N
Formula: C17H26O3
SMILES: C=C1C(OC(C)=O)C(O)C2C3C1C2(C)CCCC3(C)C
Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
gf	-109.17	kJ/mol	Joback Method
hf	-551.80	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	75.97	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.927		Crippen Method
mcvol	226.820	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	766.55	K	Joback Method
tc	973.83	K	Joback Method
tf	505.63	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.67	J/mol×K	766.55	Joback Method
cpg	763.00	J/mol×K	801.10	Joback Method
cpg	782.03	J/mol×K	835.64	Joback Method
cpg	800.96	J/mol×K	870.19	Joback Method
cpg	820.00	J/mol×K	904.73	Joback Method
cpg	839.34	J/mol×K	939.28	Joback Method
cpg	859.20	J/mol×K	973.83	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=R626396&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