3«beta»-acetoxy manoyl oxide

Inchi: InChI=1S/C22H36O3/c1-8-20(5)13-10-16-21(6)12-9-11-19(3,4)17(21)14-18(24-15(2)23)2
InchiKey: CTROLPKOIMLOHG-BYFCMQGQSA-N
Formula: C22H36O3
SMILES: C=CC1(C)CCC2C3(C)CCCC(C)(C)C3CC(OC(C)=O)C2(C)O1
Mol. weight [g/mol]: 348.52

Physical Properties

Property code	Value	Unit	Source
gf	-28.89	kJ/mol	Joback Method
hf	-581.58	kJ/mol	Joback Method
hfus	25.22	kJ/mol	Joback Method
hvap	72.32	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.284		Crippen Method
mcvol	297.270	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2376.00		NIST Webbook
tb	826.53	K	Joback Method
tc	1061.68	K	Joback Method
tf	549.53	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.62	J/mol×K	826.53	Joback Method
cpg	1043.68	J/mol×K	865.72	Joback Method
cpg	1074.67	J/mol×K	904.91	Joback Method
cpg	1107.11	J/mol×K	944.11	Joback Method
cpg	1141.53	J/mol×K	983.30	Joback Method
cpg	1178.43	J/mol×K	1022.49	Joback Method
cpg	1218.33	J/mol×K	1061.68	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=R333450&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