ent-3«beta»-acetoxy-13-epi-manoyl oxide

Inchi: InChI=1S/C22H36O3/c1-8-20(5)12-9-17-21(6)13-11-18(24-15(2)23)19(3,4)16(21)10-14-2
InchiKey: XMEKIZPKINZLRR-HTGCZIDLSA-N
Formula: C22H36O3
SMILES: C=CC1(C)CCC2C(C)(CCC3C(C)(C)C(OC(C)=O)CCC23C)O1
Mol. weight [g/mol]: 348.52

Physical Properties

Property code	Value	Unit	Source
hfus	25.22	kJ/mol	Joback Method
logp	5.284		Crippen Method
mcvol	297.270	ml/mol	McGowan Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook
ripol	2748.00		NIST Webbook
ripol	2748.00		NIST Webbook

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R327638&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices