16-Acetoxycarterochaetol

Inchi: InChI=1S/C21H34O4/c1-14(8-12-22)16-13-18-19(3)9-6-10-20(4,24-15(2)23)17(19)7-11-2
InchiKey: KIXPERSNBXFRMS-DEWOUJRRSA-N
Formula: C21H34O4
SMILES: CC(=O)OC1(C)CCCC2(C)C1CCC1(C)OC(C(C)=CCO)CC12
Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-165.00	kJ/mol	Joback Method
hf	-719.91	kJ/mol	Joback Method
hfus	34.22	kJ/mol	Joback Method
hvap	88.77	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.011		Crippen Method
mcvol	289.050	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	2787.00		NIST Webbook
rinpol	2787.00		NIST Webbook
tb	903.35	K	Joback Method
tc	1126.00	K	Joback Method
tf	565.66	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.35	J/mol×K	903.35	Joback Method
cpg	1059.59	J/mol×K	940.46	Joback Method
cpg	1088.00	J/mol×K	977.57	Joback Method
cpg	1117.94	J/mol×K	1014.68	Joback Method
cpg	1149.80	J/mol×K	1051.79	Joback Method
cpg	1183.94	J/mol×K	1088.89	Joback Method
cpg	1220.74	J/mol×K	1126.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R604227&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