16-Acetoxycarterochaetol

Inchi: InChI=1S/C22H36O3/c1-15(9-13-24-16(2)23)17-14-19-21(5)11-7-10-20(3,4)18(21)8-12-2
InchiKey: XJXXRCYCZWSCRN-WSFUHMCBSA-N
Formula: C22H36O3
SMILES: CC(=O)OCC=C(C)C1CC2C(C)(CCC3C(C)(C)CCCC32C)O1
Mol. weight [g/mol]: 348.52

Physical Properties

Property code	Value	Unit	Source
gf	-19.76	kJ/mol	Joback Method
hf	-588.32	kJ/mol	Joback Method
hfus	32.72	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.286		Crippen Method
mcvol	297.270	ml/mol	McGowan Method
pc	1361.64	kPa	Joback Method
rinpol	2787.00		NIST Webbook
rinpol	2787.00		NIST Webbook
tb	834.05	K	Joback Method
tc	1063.58	K	Joback Method
tf	516.11	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1012.54	J/mol×K	834.05	Joback Method
cpg	1040.35	J/mol×K	872.31	Joback Method
cpg	1068.62	J/mol×K	910.56	Joback Method
cpg	1097.76	J/mol×K	948.82	Joback Method
cpg	1128.17	J/mol×K	987.07	Joback Method
cpg	1160.27	J/mol×K	1025.33	Joback Method
cpg	1194.46	J/mol×K	1063.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R587276&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

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