14-Acetoxy-4,5-epoxy-«beta»-caryophyllene («beta»«alpha»)

Other names: 14-Acetoxy-4,5-epoxy- «beta»-caryophyllene
Inchi: InChI=1S/C17H26O3/c1-11-5-6-15-17(20-15,10-19-12(2)18)8-7-14-13(11)9-16(14,3)4/h1
InchiKey: BDESUTAYQPYKDJ-UHFFFAOYSA-N
Formula: C17H26O3
SMILES: C=C1CCC2OC2(COC(C)=O)CCC2C1CC2(C)C
Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
gf	-55.15	kJ/mol	Joback Method
hf	-497.05	kJ/mol	Joback Method
hfus	27.04	kJ/mol	Joback Method
hvap	64.60	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.480		Crippen Method
mcvol	226.820	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
ripol	2617.00		NIST Webbook
ripol	2617.00		NIST Webbook
ripol	2617.00		NIST Webbook
ripol	2617.00		NIST Webbook
ripol	2617.00		NIST Webbook
tb	714.93	K	Joback Method
tc	939.38	K	Joback Method
tf	476.34	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.01	J/mol×K	714.93	Joback Method
cpg	727.44	J/mol×K	752.34	Joback Method
cpg	748.17	J/mol×K	789.75	Joback Method
cpg	768.46	J/mol×K	827.16	Joback Method

cpg	788.57	J/mol×K	864.57	Joback Method
cpg	808.77	J/mol×K	901.97	Joback Method
cpg	829.32	J/mol×K	939.38	Joback Method

Sources

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=R336142&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume