12-Acetoxycaryophyllene-4,5-epoxide

Inchi: InChI=1S/C17H28O3/c1-11(18)19-10-12-5-6-15-17(4,20-15)8-7-14-13(12)9-16(14,2)3/h1
InchiKey: JXTAVNIIVRAIGB-UHFFFAOYSA-N
Formula: C17H28O3
SMILES: CC(=O)OCC1CCC2OC2(C)CCC2C1CC2(C)C
Mol. weight [g/mol]: 280.40

Physical Properties

Property code	Value	Unit	Source
gf	-115.94	kJ/mol	Joback Method
hf	-601.63	kJ/mol	Joback Method
hfus	29.27	kJ/mol	Joback Method
hvap	64.13	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.559		Crippen Method
mcvol	231.120	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook
tb	711.10	K	Joback Method
tc	933.95	K	Joback Method
tf	458.42	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.75	J/mol×K	711.10	Joback Method
cpg	756.55	J/mol×K	748.24	Joback Method
cpg	778.53	J/mol×K	785.38	Joback Method
cpg	799.95	J/mol×K	822.52	Joback Method
cpg	821.06	J/mol×K	859.66	Joback Method
cpg	842.13	J/mol×K	896.80	Joback Method
cpg	863.42	J/mol×K	933.95	Joback Method

Sources

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=R226941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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