6-Acetoxycaryophyllene

Inchi: InChI=1S/C17H26O2/c1-11-6-7-16-15(10-17(16,4)5)12(2)9-14(8-11)19-13(3)18/h8,14-16
InchiKey: OJBFJKMLUPVZDL-LKUCEOIBSA-N
Formula: C17H26O2
SMILES: C=C1CC(OC(C)=O)C=C(C)CCC2C1CC2(C)C
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-28.16	kJ/mol	Joback Method
hf	-419.10	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	62.62	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.267		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
ripol	2210.00		NIST Webbook
ripol	2210.00		NIST Webbook
ripol	2210.00		NIST Webbook
tb	693.68	K	Joback Method
tc	915.09	K	Joback Method
tf	414.17	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.67	J/mol×K	693.68	Joback Method
cpg	693.69	J/mol×K	730.58	Joback Method
cpg	714.56	J/mol×K	767.48	Joback Method
cpg	734.39	J/mol×K	804.38	Joback Method
cpg	753.29	J/mol×K	841.28	Joback Method
cpg	771.37	J/mol×K	878.19	Joback Method
cpg	788.75	J/mol×K	915.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R340606&Units=SI

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