«alpha»-caryophylene acetate

Inchi: InChI=1S/C17H26O2/c1-13-8-9-16(19-15(3)18)14(2)7-6-11-17(4,5)12-10-13/h6,10-11,16
InchiKey: KNKUCEKTTLJYCQ-PIUHNEHMSA-N
Formula: C17H26O2
SMILES: C=C1CC=CC(C)(C)CC=C(C)CCC1OC(C)=O
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-87.54	kJ/mol	Joback Method
hf	-432.26	kJ/mol	Joback Method
hfus	19.58	kJ/mol	Joback Method
hvap	63.83	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.577		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1686.20		NIST Webbook
rinpol	1686.20		NIST Webbook
tb	703.58	K	Joback Method
tc	933.00	K	Joback Method
tf	390.67	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.47	J/mol×K	703.58	Joback Method
cpg	692.05	J/mol×K	741.82	Joback Method
cpg	713.35	J/mol×K	780.05	Joback Method
cpg	733.42	J/mol×K	818.29	Joback Method
cpg	752.34	J/mol×K	856.53	Joback Method
cpg	770.18	J/mol×K	894.76	Joback Method
cpg	787.02	J/mol×K	933.00	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=R283102&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume