Caryophyllene acetate

Other names:	acetoxy-caryophyllene
Inchi:	[1R-(1«alpha»,2«alpha»,5«beta»,8«beta»)]-4,4,8-trimethyltricyclo[6.3.1.02,5]dodecan-1-yl acetate InChI=1S/C17H28O2/c1-12(18)19-17-8-5-7-16(4,11-17)9-6-13-14(17)10-15(13,2)3/h13-1
InchiKey:	SJDDHMSVZMBJPH-UHFFFAOYSA-N
Formula:	C17H28O2
SMILES:	CC(=O)OC12CCCC(C)(CCC3C1CC3(C)C)C2
Mol. weight [g/mol]:	264.40
CAS:	57082-24-3

Physical Properties

Property code	Value	Unit	Source
gf	-27.60	kJ/mol	Joback Method
hf	-434.05	kJ/mol	Joback Method
hfus	13.93	kJ/mol	Joback Method
hvap	58.78	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.325		Crippen Method
mcvol	225.250	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1708.30		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1690.00		NIST Webbook
tb	689.06	K	Joback Method
tc	922.50	K	Joback Method
tf	459.99	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	691.73	J/mol×K	689.06	Joback Method
cpg	715.17	J/mol×K	727.97	Joback Method
cpg	737.95	J/mol×K	766.87	Joback Method
cpg	760.48	J/mol×K	805.78	Joback Method
cpg	783.18	J/mol×K	844.68	Joback Method
cpg	806.47	J/mol×K	883.59	Joback Method
cpg	830.75	J/mol×K	922.50	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=C57082243&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

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