Bicyclo[3.1.1]hept-2-en-6-ol, 2,7,7-trimethyl-, acetate, [1S-(1«alpha»,5«alpha»,6«beta»)]-

Other names:	(+)-trans-Chrysanthenyl acetate
	trans-Chrysanthenyl acetate
	Bicyclo[3.1.1]hept-2-en-6-ol, 2,7,7-trimethyl-, acetate, (1S,5R,6R)-
	2,7,7-Trimethylbicyclo[3.1.1]hept-2-en-6-yl, acetate, [1S-(1«alpha»,5«alpha»,6«beta»)]-
	trans-Chrisanthenyl acetate
Inchi:	InChI=1S/C12H18O2/c1-7-5-6-9-11(14-8(2)13)10(7)12(9,3)4/h5,9-11H,6H2,1-4H3
InchiKey:	UASZOTVHPVEMQR-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	CC(=O)OC1C2CC=C(C)C1C2(C)C
Mol. weight [g/mol]:	194.27
CAS:	50764-55-1

Physical Properties

Property code	Value	Unit	Source
gf	-74.94	kJ/mol	Joback Method
hf	-375.50	kJ/mol	Joback Method
hfus	20.47	kJ/mol	Joback Method
hvap	50.64	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1242.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1237.90		NIST Webbook
tb	563.04	K	Joback Method
tc	773.40	K	Joback Method
tf	358.22	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.92	J/mol×K	563.04	Joback Method

cpg	437.32	J/mol×K	598.10	Joback Method
cpg	453.71	J/mol×K	633.16	Joback Method
cpg	469.20	J/mol×K	668.22	Joback Method
cpg	483.90	J/mol×K	703.28	Joback Method
cpg	497.94	J/mol×K	738.34	Joback Method
cpg	511.43	J/mol×K	773.40	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=C50764551&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

Latest version available from:
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