Myrtenyl acetate

Other names:	2-Pinen-10-ol, acetate
	Bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-, acetate, (1S)-
	(1S)-6,6-Dimethylbicyclo(3.1.1)hept-2-ene-2-methanol acetate
	(+)-Myrtenyl acetate
	myrtenalacetate
	(1S)-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)methyl acetate
Inchi:	InChI=1S/C12H18O2/c1-8(13)14-7-9-4-5-10-6-11(9)12(10,2)3/h4,10-11H,5-7H2,1-3H3
InchiKey:	BKATZVAUANSCKN-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	CC(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]:	194.27
CAS:	1079-01-2

Physical Properties

Property code	Value	Unit	Source
gf	-67.23	kJ/mol	Joback Method
hf	-355.16	kJ/mol	Joback Method
hfus	19.40	kJ/mol	Joback Method
hvap	50.95	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.542		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1312.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1297.00		NIST Webbook

rinpol	1327.00	NIST Webbook
rinpol	1326.00	NIST Webbook
rinpol	1293.00	NIST Webbook
rinpol	1320.00	NIST Webbook
rinpol	1299.00	NIST Webbook
rinpol	1304.00	NIST Webbook
rinpol	1310.00	NIST Webbook
rinpol	1324.00	NIST Webbook
rinpol	1307.00	NIST Webbook
rinpol	1284.00	NIST Webbook
rinpol	1322.00	NIST Webbook
rinpol	1325.00	NIST Webbook
rinpol	1327.00	NIST Webbook
rinpol	1299.00	NIST Webbook
rinpol	1306.00	NIST Webbook
rinpol	1328.00	NIST Webbook
rinpol	1301.00	NIST Webbook
rinpol	1307.00	NIST Webbook
rinpol	1300.00	NIST Webbook
rinpol	1306.00	NIST Webbook
rinpol	1306.00	NIST Webbook
rinpol	1301.00	NIST Webbook
rinpol	1326.80	NIST Webbook
rinpol	1336.90	NIST Webbook
rinpol	1336.00	NIST Webbook
rinpol	1332.00	NIST Webbook
rinpol	1324.00	NIST Webbook
rinpol	1335.00	NIST Webbook
rinpol	1304.00	NIST Webbook
rinpol	1332.00	NIST Webbook
rinpol	1285.00	NIST Webbook
rinpol	1324.00	NIST Webbook
rinpol	1285.00	NIST Webbook
rinpol	1323.00	NIST Webbook
rinpol	1335.00	NIST Webbook
rinpol	1332.00	NIST Webbook
rinpol	1332.00	NIST Webbook
ripol	1720.00	NIST Webbook
ripol	1704.00	NIST Webbook
ripol	1704.00	NIST Webbook
ripol	1698.00	NIST Webbook
ripol	1698.00	NIST Webbook
ripol	1720.00	NIST Webbook
ripol	1698.00	NIST Webbook

ripol	1698.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1677.00		NIST Webbook
ripol	1707.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1704.00		NIST Webbook
tb	567.71	K	Joback Method
tc	778.17	K	Joback Method
tf	362.46	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.70	J/mol×K	567.71	Joback Method
cpg	435.64	J/mol×K	602.79	Joback Method
cpg	451.57	J/mol×K	637.86	Joback Method
cpg	466.60	J/mol×K	672.94	Joback Method
cpg	480.88	J/mol×K	708.02	Joback Method
cpg	494.51	J/mol×K	743.09	Joback Method
cpg	507.64	J/mol×K	778.17	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=C1079012&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume