Bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, acetate

Other names: 4(10)-Thujen-3-ol, acetate
Sabinyl acetate
«beta»-Sabinyl acetate

Inchi: InChI=1S/C12H18O2/c1-7(2)12-5-10(12)8(3)11(6-12)14-9(4)13/h7,10-11H,3,5-6H2,1-2,4

InchiKey: PBWRFXQNNGSAQG-UHFFFAOYSA-N

Formula: C12H18O2

SMILES: C=C1C(OC(C)=O)CC2(C(C)C)CC12

Mol. weight [g/mol]: 194.27

CAS: 3536-54-7

Physical Properties

Property code	Value	Unit	Source
gf	-24.82	kJ/mol	Joback Method
hf	-316.35	kJ/mol	Joback Method
hfus	15.98	kJ/mol	Joback Method
hvap	49.60	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	1295.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1288.00		NIST Webbook

rinpol	1289.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1291.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1658.00		NIST Webbook
tb	558.02	K	Joback Method
tc	764.52	K	Joback Method
tf	351.38	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.14	J/mol×K	558.02	Joback Method
cpg	433.79	J/mol×K	592.44	Joback Method
cpg	449.43	J/mol×K	626.85	Joback Method
cpg	464.18	J/mol×K	661.27	Joback Method
cpg	478.16	J/mol×K	695.68	Joback Method
cpg	491.51	J/mol×K	730.10	Joback Method
cpg	504.33	J/mol×K	764.52	Joback Method

Sources

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=C3536547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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