

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	1266.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1289.00		NIST Webbook

ripol	1276.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1301.00		NIST Webbook
ripol	1263.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1658.00		NIST Webbook
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ripol	1651.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1665.00		NIST Webbook
tb	558.02	K	Joback Method
tc	764.52	K	Joback Method
tf	351.38	K	Joback Method
vc	0.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3536547&Units=SI

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r_{in}pol:	Non-polar retention indices
r_{ip}ol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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