Bicyclo[3.1.1]hept-2-en-4-ol, 2,6,6-trimethyl-, acetate

Other names: verbenyl acetate
verbenol acetate

Inchi: InChI=1S/C12H18O2/c1-7-5-11(14-8(2)13)10-6-9(7)12(10,3)4/h5,9-11H,6H2,1-4H3

InchiKey: OZBFUQLOVFXDNK-UHFFFAOYSA-N

Formula: C12H18O2

SMILES: CC(=O)OC1C=C(C)C2CC1C2(C)C

Mol. weight [g/mol]: 194.27

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	1297.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1282.00		NIST Webbook
ripol	1690.00		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: 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=U195660&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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