4-Thujen-2-«alpha»-yl acetate

Other names: Sabinil acetate trans
Inchi: InChI=1S/C12H18O2/c1-7(2)12-6-10(12)8(3)5-11(12)14-9(4)13/h5,7,10-11H,6H2,1-4H3
InchiKey: OIAIPKLZAGWFDB-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CC(=O)OC1C=C(C)C2CC12C(C)C
Mol. weight [g/mol]: 194.27
CAS: 53833-85-5

Physical Properties

Property code	Value	Unit	Source
gf	-57.57	kJ/mol	Joback Method
hf	-354.28	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	50.39	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1277.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1275.00		NIST Webbook
tb	563.00	K	Joback Method
tc	770.72	K	Joback Method
tf	350.98	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.04	J/mol×K	563.00	Joback Method
cpg	434.48	J/mol×K	597.62	Joback Method
cpg	449.93	J/mol×K	632.24	Joback Method
cpg	464.51	J/mol×K	666.86	Joback Method

cpg	478.34	J/mol×K	701.48	Joback Method
cpg	491.55	J/mol×K	736.10	Joback Method
cpg	504.28	J/mol×K	770.72	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=C53833855&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume