(Z)-Pinocarvyl acetate

Inchi: InChI=1S/C12H18O2/c1-7-10-5-9(12(10,3)4)6-11(7)14-8(2)13/h9-11H,1,5-6H2,2-4H3/t9-
InchiKey: UDBAGFUFASPUFS-OUAUKWLOSA-N
Formula: C12H18O2
SMILES: C=C1C(OC(C)=O)CC2CC1C2(C)C
Mol. weight [g/mol]: 194.27
CAS: 73366-18-4

Physical Properties

Property code	Value	Unit	Source
gf	-42.19	kJ/mol	Joback Method
hf	-337.57	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	49.85	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook
tb	558.06	K	Joback Method
tc	767.19	K	Joback Method
tf	358.62	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.91	J/mol×K	558.06	Joback Method
cpg	436.52	J/mol×K	592.92	Joback Method
cpg	453.10	J/mol×K	627.77	Joback Method
cpg	468.76	J/mol×K	662.63	Joback Method
cpg	483.62	J/mol×K	697.48	Joback Method
cpg	497.79	J/mol×K	732.34	Joback Method
cpg	511.38	J/mol×K	767.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73366184&Units=SI
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

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