(Z)-«alpha»-Santalyl acetate

Inchi: InChI=1S/C17H26O2/c1-11(10-19-12(2)18)6-5-7-16(3)13-8-14-15(9-13)17(14,16)4/h6,13
InchiKey: IXRPKRWXUJOOBZ-IZZDOVSWSA-N
Formula: C17H26O2
SMILES: CC(=O)OCC(C)=CCCC1(C)C2CC3C(C2)C31C
Mol. weight [g/mol]: 262.39
CAS: 41414-75-9

Physical Properties

Property code	Value	Unit	Source
gf	110.06	kJ/mol	Joback Method
hf	-311.06	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	59.11	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.958		Crippen Method
mcvol	220.950	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	1788.00		NIST Webbook
rinpol	1773.00		NIST Webbook
tb	671.51	K	Joback Method
tc	876.44	K	Joback Method
tf	434.65	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.79	J/mol×K	671.51	Joback Method
cpg	677.42	J/mol×K	705.66	Joback Method
cpg	695.36	J/mol×K	739.82	Joback Method
cpg	712.87	J/mol×K	773.97	Joback Method
cpg	730.22	J/mol×K	808.13	Joback Method
cpg	747.66	J/mol×K	842.28	Joback Method
cpg	765.44	J/mol×K	876.44	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41414759&Units=SI

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