(E)-«beta»-Santalol acetate

Other names: (E)-«beta»-Santalyl acetate
Inchi: InChI=1S/C17H26O2/c1-12(11-19-14(3)18)6-5-9-17(4)13(2)15-7-8-16(17)10-15/h6,15-16
InchiKey: RCFGRZLLBGMERD-DQRCMHBESA-N
Formula: C17H26O2
SMILES: C=C1C2CCC(C2)C1(C)CCC=C(C)COC(C)=O
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	79.29	kJ/mol	Joback Method
hf	-313.00	kJ/mol	Joback Method
hfus	29.25	kJ/mol	Joback Method
hvap	61.33	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.268		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	681.17	K	Joback Method
tc	886.42	K	Joback Method
tf	400.17	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.97	J/mol×K	681.17	Joback Method
cpg	678.12	J/mol×K	715.38	Joback Method
cpg	696.38	J/mol×K	749.59	Joback Method

cpg	713.90	J/mol×K	783.80	Joback Method
cpg	730.81	J/mol×K	818.00	Joback Method
cpg	747.25	J/mol×K	852.21	Joback Method
cpg	763.38	J/mol×K	886.42	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=R129954&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