epi-«beta»-Santalol, 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-UTLCUASFSA-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	1799.00		NIST Webbook
rinpol	1799.00		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R129989&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

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