«alpha»-Bisabolol acetate

Inchi: InChI=1S/C17H28O2/c1-13(2)7-6-12-17(5,19-15(4)18)16-10-8-14(3)9-11-16/h7-8,16H,6,
InchiKey: RQYNNIWGGJJGDH-IAGOWNOFSA-N
Formula: C17H28O2
SMILES: CC(=O)OC(C)(CCC=C(C)C)C1CC=C(C)CC1
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	-22.37	kJ/mol	Joback Method
hf	-439.70	kJ/mol	Joback Method
hfus	26.72	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.801		Crippen Method
mcvol	238.370	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	689.15	K	Joback Method
tc	898.62	K	Joback Method
tf	357.55	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.46	J/mol×K	689.15	Joback Method
cpg	704.69	J/mol×K	724.06	Joback Method
cpg	723.65	J/mol×K	758.97	Joback Method
cpg	741.42	J/mol×K	793.88	Joback Method
cpg	758.06	J/mol×K	828.80	Joback Method
cpg	773.62	J/mol×K	863.71	Joback Method
cpg	788.17	J/mol×K	898.62	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=R608303&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