«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-UHFFFAOYSA-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	1786.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1786.00		NIST Webbook
rinpol	1786.00		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

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=R129721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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