trans-«alpha»-Bergamotol acetate

Inchi: InChI=1S/C17H26O2/c1-12(11-19-14(3)18)6-5-9-17(4)15-8-7-13(2)16(17)10-15/h6-7,15-
InchiKey: BDYQEBZJCFGMCH-MSMUUXKQSA-N
Formula: C17H26O2
SMILES: CC(=O)OCC(C)=CCCC1(C)C2CC=C(C)C1C2
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	46.54	kJ/mol	Joback Method
hf	-350.93	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	62.12	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.268		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	1800.00		NIST Webbook
tb	686.15	K	Joback Method
tc	892.39	K	Joback Method
tf	399.77	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.76	J/mol×K	686.15	Joback Method
cpg	678.74	J/mol×K	720.52	Joback Method
cpg	696.87	J/mol×K	754.90	Joback Method
cpg	714.28	J/mol×K	789.27	Joback Method
cpg	731.12	J/mol×K	823.64	Joback Method
cpg	747.53	J/mol×K	858.02	Joback Method
cpg	763.66	J/mol×K	892.39	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=R234185&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