(E)-«alpha»-Santalol

Inchi: InChI=1S/C15H24O/c1-10(9-16)5-4-6-14(2)11-7-12-13(8-11)15(12,14)3/h5,11-13,16H,4,
InchiKey: PDEQKAVEYSOLJX-LPUUACFHSA-N
Formula: C15H24O
SMILES: CC(=CCCC1(C)C2CC3C(C2)C31C)CO
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	190.32	kJ/mol	Joback Method
hf	-177.21	kJ/mol	Joback Method
hfus	25.74	kJ/mol	Joback Method
hvap	62.18	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.387		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
ripol	1742.00		NIST Webbook
tb	641.64	K	Joback Method
tc	834.93	K	Joback Method
tf	400.77	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.45	J/mol×K	641.64	Joback Method
cpg	582.63	J/mol×K	673.86	Joback Method
cpg	598.08	J/mol×K	706.07	Joback Method
cpg	613.05	J/mol×K	738.29	Joback Method
cpg	627.75	J/mol×K	770.50	Joback Method
cpg	642.41	J/mol×K	802.72	Joback Method
cpg	657.26	J/mol×K	834.93	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=R634921&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume