(Z)-«beta»-Santalol

Inchi: InChI=1S/C15H24O/c1-11(10-16)5-4-6-15(3)12(2)7-13-8-14(15)9-13/h5,13-14,16H,2,4,6-
InchiKey: VTXPWIQSFDTJNV-WZUFQYTHSA-N
Formula: C15H24O
SMILES: C=C1CC2CC(C2)C1(C)CCC=C(C)CO
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	159.55	kJ/mol	Joback Method
hf	-179.15	kJ/mol	Joback Method
hfus	25.37	kJ/mol	Joback Method
hvap	64.40	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1716.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1716.00		NIST Webbook
ripol	1692.00		NIST Webbook
tb	651.30	K	Joback Method
tc	845.06	K	Joback Method
tf	366.29	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.45	J/mol×K	651.30	Joback Method
cpg	582.25	J/mol×K	683.59	Joback Method
cpg	598.24	J/mol×K	715.89	Joback Method
cpg	613.56	J/mol×K	748.18	Joback Method
cpg	628.33	J/mol×K	780.48	Joback Method
cpg	642.69	J/mol×K	812.77	Joback Method

cpg	656.76	J/mol×K	845.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R625195&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume