«beta»-Santalol

Other names:	Beta-santalol
	«beta»-Santalol (Z)
	2-Penten-1-ol, 2-methyl-5-(2-methyl-3-methylenebicyclo[2.2.1]hept-2-yl)-, [1S-[1«alpha»,2«alpha»(Z),4«alpha»]]-
	«beta»-(Z)-Santalol
	(Z)-«beta»-Santalol
	2-Penten-1-ol, 2-methyl-5-[(1S,2R,4R)-2-methyl-3-methylenebicyclo[2.2.1]hept-2-yl]-, (2Z)-
	(2Z)-2-Methyl-5-((1S,2R,4R)-2-methyl-3-methylenebicyclo[2.2.1]hept-2-yl)-2-penten-1-ol
	[1S-[1«alpha»,2«alpha»(Z),4«alpha»]]-2-methyl-5-(2-methyl-3-methylenebicyclo[2.2.1]hep
Inchi:	InChI=1S/C15H24O/c1-11(10-16)5-4-8-15(3)12(2)13-6-7-14(15)9-13/h5,13-14,16H,2,4,6-
InchiKey:	OJYKYCDSGQGTRJ-AKZWGNFOSA-N
Formula:	C15H24O
SMILES:	C=C1C2CCC(C2)C1(C)CCC=C(C)CO
Mol. weight [g/mol]:	220.35
CAS:	77-42-9

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	1678.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1723.90		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1680.00		NIST Webbook

rinpol	1694.00		NIST Webbook
rinpol	1720.00		NIST Webbook
ripol	2391.00		NIST Webbook
ripol	2434.00		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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77429&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

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