«alpha»-Santalol

Other names:	2-Penten-1-ol, 5-(2,3-dimethyltricyclo[2.2.1.0(2,6)]hept-3-yl)-2-methyl-, [R(Z)]-
	(+)-«alpha»-Santalol
	cis-«alpha»-Santalol
	Sandal
	Santalol A
	d-«alpha»-Santalol
	alpha-Santalol
	(Z)- «alpha»-Santalool
	«alpha»-Santanol
	5-(2,3-dimethyltricyclo[2.2.1.02,6]hept-3-yl)-2-methylpent-2-en-1-ol, stereoisomer
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-NVFXPZDQSA-N
Formula:	C15H24O
SMILES:	CC(=CCCC1(C)C2CC3C(C2)C31C)CO
Mol. weight [g/mol]:	220.35
CAS:	115-71-9

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
rinpol	1669.00		NIST Webbook
rinpol	1681.10		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1682.90		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1660.00		NIST Webbook

rinpol	1660.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1682.90		NIST Webbook
rinpol	1672.80		NIST Webbook
rinpol	1676.00		NIST Webbook
ripol	1843.00		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
hvapt	58.30	kJ/mol	371.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.20	K	1.90	NIST Webbook

Sources

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=C115719&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume