

(E)-«beta»-Santalol

Other names:	Santalol <E,«BETA»> «beta»-trans-santalol «beta»-(E)-Santalol
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-PIDYCISJSA-N
Formula:	C15H24O
SMILES:	C=C1C2CCC(C2)C1(C)CCC=C(C)CO
Mol. weight [g/mol]:	220.35
CAS:	37172-32-0

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	1731.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1744.80		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1738.00		NIST Webbook
rinpol	1744.00		NIST Webbook
tb	651.30	K	Joback Method
tc	845.06	K	Joback Method
tf	366.29	K	Joback Method
vc	0.762	m ³ /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

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=C37172320&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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