

(Z)-Santalol

Inchi:	InChI=1S/C15H24O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16/h2-9,16H,10-15H2,1H3/b3
InchiKey:	RAPKQMZFSCMPDF-FUKINOADSA-N
Formula:	C15H24O
SMILES:	CC=CC=CC=CC=CCCCCCO
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	259.48	kJ/mol	Joback Method
hf	-36.28	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	65.50	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.174		Crippen Method
mcvol	210.880	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook
tb	651.42	K	Joback Method
tc	829.59	K	Joback Method
tf	299.31	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.90	J/molxK	651.42	Joback Method
cpg	618.79	J/molxK	799.90	Joback Method
cpg	606.82	J/molxK	770.20	Joback Method
cpg	594.31	J/molxK	740.51	Joback Method
cpg	581.18	J/molxK	710.81	Joback Method
cpg	567.40	J/molxK	681.12	Joback Method
cpg	630.27	J/molxK	829.59	Joback Method
dvisc	0.0000256	Paxs	651.42	Joback Method

dvisc	0.0000425	Paxs	592.74	Joback Method
dvisc	0.0000791	Paxs	534.05	Joback Method
dvisc	0.0001715	Paxs	475.37	Joback Method
dvisc	0.0004623	Paxs	416.68	Joback Method
dvisc	0.0017253	Paxs	358.00	Joback Method
dvisc	0.0107907	Paxs	299.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R586268&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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