«beta»-(Z)-Santalol

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-YHYXMXQVSA-N
Formula: C15H24O
SMILES: CC(=CCCC1(C)C2CC3C(C2)C31C)CO
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	25.74	kJ/mol	Joback Method
logp	3.387		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
rinpol	1713.00		NIST Webbook
rinpol	1713.00		NIST Webbook

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

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R616869&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices