(Z)-«alpha»-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	1665.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1669.00		NIST Webbook
ripol	2306.00		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=R601837&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
ripol:	Polar retention indices

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