Isolongifolol

Inchi: InChI=1S/C15H26O/c1-12(2)7-5-8-15(16)13(3,4)11-6-9-14(12,15)10-11/h11,16H,5-10H2
InchiKey: CCMWYZQSEJEAEY-NFCBODTESA-N
Formula: C15H26O
SMILES: CC1(C)CCCC2(O)C(C)(C)C3CCC12C3
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	5.85	kJ/mol	Joback Method
logp	3.754		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
rinpol	1740.90		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1740.90		NIST Webbook
ripol	2219.00		NIST Webbook
ripol	2219.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.59	J/mol×K	655.16	Joback Method
cpg	610.07	J/mol×K	692.02	Joback Method
cpg	629.03	J/mol×K	728.88	Joback Method
cpg	647.94	J/mol×K	765.73	Joback Method
cpg	667.27	J/mol×K	802.59	Joback Method
cpg	687.47	J/mol×K	839.45	Joback Method
cpg	709.02	J/mol×K	876.31	Joback Method

Sources

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=R185003&Units=SI
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

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