Longifolol

Inchi: InChI=1S/C15H26O/c1-14(2)7-4-8-15(3)11-6-5-10(13(11)14)12(15)9-16/h10-13,16H,4-9H
InchiKey: VZJHQHUOVIDRCF-JCMLLNEPSA-N
Formula: C15H26O
SMILES: CC1(C)CCCC2(C)C(CO)C3CCC2C31
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	62.54	kJ/mol	Joback Method
hf	-329.62	kJ/mol	Joback Method
hfus	19.52	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.467		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	650.01	K	Joback Method
tc	856.17	K	Joback Method
tf	401.49	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.04	J/mol×K	650.01	Joback Method
cpg	619.09	J/mol×K	684.37	Joback Method
cpg	638.22	J/mol×K	718.73	Joback Method
cpg	656.66	J/mol×K	753.09	Joback Method
cpg	674.65	J/mol×K	787.45	Joback Method
cpg	692.39	J/mol×K	821.81	Joback Method
cpg	710.12	J/mol×K	856.17	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=R430145&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