(-)-Isolongifolol, methyl ether

Inchi: InChI=1S/C16H28O/c1-15(2)8-5-9-16(3)12-7-6-11(14(12)15)13(16)10-17-4/h11-14H,5-10
InchiKey: GDVBDGSQRFXTGJ-UHFFFAOYSA-N
Formula: C16H28O
SMILES: COCC1C2CCC3C2C(C)(C)CCCC13C
Mol. weight [g/mol]: 236.39

Physical Properties

Property code	Value	Unit	Source
gf	102.78	kJ/mol	Joback Method
hf	-330.25	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	50.47	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	4.121		Crippen Method
mcvol	209.590	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	1671.70		NIST Webbook
rinpol	1671.70		NIST Webbook
tb	603.13	K	Joback Method
tc	818.80	K	Joback Method
tf	374.17	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.88	J/mol×K	603.13	Joback Method
cpg	632.12	J/mol×K	639.07	Joback Method
cpg	654.99	J/mol×K	675.02	Joback Method
cpg	676.75	J/mol×K	710.96	Joback Method
cpg	697.63	J/mol×K	746.91	Joback Method
cpg	717.89	J/mol×K	782.85	Joback Method
cpg	737.75	J/mol×K	818.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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