11-epi-Eudesma-4(15),7-dien-12-yl methyl ether

Inchi: InChI=1S/C16H26O/c1-12-6-5-8-16(3)9-7-14(10-15(12)16)13(2)11-17-4/h7,13,15H,1,5-6
InchiKey: JGJVWKKEHVYBGK-AVVWSFFYSA-N
Formula: C16H26O
SMILES: C=C1CCCC2(C)CC=C(C(C)COC)CC12
Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	117.42	kJ/mol	Joback Method
hf	-244.32	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	53.71	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	4.352		Crippen Method
mcvol	211.850	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
ripol	2000.00		NIST Webbook
ripol	2000.00		NIST Webbook
tb	621.56	K	Joback Method
tc	837.74	K	Joback Method
tf	349.97	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.66	J/mol×K	621.56	Joback Method
cpg	604.66	J/mol×K	657.59	Joback Method
cpg	625.45	J/mol×K	693.62	Joback Method
cpg	645.17	J/mol×K	729.65	Joback Method
cpg	663.93	J/mol×K	765.68	Joback Method
cpg	681.87	J/mol×K	801.71	Joback Method

cpg	699.11	J/mol×K	837.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R236012&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume