4-«beta»-H-cis-Eudesma-6,11-dien-3-«beta»-yl methyl ether

Inchi: InChI=1S/C16H26O/c1-11(2)13-6-8-16(4)9-7-15(17-5)12(3)14(16)10-13/h10,12,14-15H,1

InchiKey: BZESABUEMVPDAR-OHRKKDJYSA-N

Formula: C16H26O

SMILES: C=C(C)C1=CC2C(C)C(OC)CCC2(C)CC1

Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	130.65	kJ/mol	Joback Method
hf	-248.32	kJ/mol	Joback Method
hfus	20.34	kJ/mol	Joback Method
hvap	52.73	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.350		Crippen Method
mcvol	211.850	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
tb	610.06	K	Joback Method
tc	828.08	K	Joback Method
tf	327.09	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.39	J/mol×K	610.06	Joback Method
cpg	607.89	J/mol×K	646.40	Joback Method
cpg	630.08	J/mol×K	682.73	Joback Method
cpg	651.09	J/mol×K	719.07	Joback Method
cpg	671.03	J/mol×K	755.41	Joback Method
cpg	690.04	J/mol×K	791.74	Joback Method
cpg	708.25	J/mol×K	828.08	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=R236072&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