Preziza-7(15)-en-12-yl methyl ether

Inchi: InChI=1S/C16H26O/c1-11-5-6-14-15(3,10-17-4)12(2)13-7-8-16(11,14)9-13/h11,13-14H,2
InchiKey: IKRCVMPMBGCISG-KWBMSBLWSA-N
Formula: C16H26O
SMILES: C=C1C2CCC3(C2)C(C)CCC3C1(C)COC
Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	163.57	kJ/mol	Joback Method
hf	-225.67	kJ/mol	Joback Method
hfus	16.98	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.042		Crippen Method
mcvol	205.290	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
ripol	2000.00		NIST Webbook
ripol	2000.00		NIST Webbook
tb	606.96	K	Joback Method
tc	824.44	K	Joback Method
tf	392.09	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.07	J/mol×K	606.96	Joback Method
cpg	607.69	J/mol×K	643.21	Joback Method
cpg	629.04	J/mol×K	679.45	Joback Method
cpg	649.38	J/mol×K	715.70	Joback Method
cpg	668.95	J/mol×K	751.95	Joback Method

cpg	688.01	J/mol×K	788.19	Joback Method
cpg	706.80	J/mol×K	824.44	Joback Method

Sources

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=R236270&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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