Preziza-7(15)-en-3a-yl methyl ether

Inchi: InChI=1S/C16H26O/c1-10-12-6-7-16(9-12)11(2)13(17-5)8-14(16)15(10,3)4/h11-14H,1,6-
InchiKey: NOKNTFRUZUWJBS-FCLZWUKPSA-N
Formula: C16H26O
SMILES: C=C1C2CCC3(C2)C(C)C(OC)CC3C1(C)C
Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	155.86	kJ/mol	Joback Method
hf	-246.01	kJ/mol	Joback Method
hfus	18.05	kJ/mol	Joback Method
hvap	50.63	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	4.040		Crippen Method
mcvol	205.290	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
ripol	1960.00		NIST Webbook
ripol	1960.00		NIST Webbook
tb	602.29	K	Joback Method
tc	819.75	K	Joback Method
tf	387.85	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.98	J/mol×K	602.29	Joback Method
cpg	609.12	J/mol×K	638.53	Joback Method
cpg	630.98	J/mol×K	674.78	Joback Method
cpg	651.78	J/mol×K	711.02	Joback Method
cpg	671.78	J/mol×K	747.26	Joback Method
cpg	691.20	J/mol×K	783.51	Joback Method
cpg	710.30	J/mol×K	819.75	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=R501410&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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