Preziza-7(15)-en-12-yl acetate

Inchi: InChI=1S/C17H26O2/c1-11-5-6-15-16(4,10-19-13(3)18)12(2)14-7-8-17(11,15)9-14/h11,1
InchiKey: PQTUSECOROEZIB-SIGHXODZSA-N
Formula: C17H26O2
SMILES: C=C1C2CCC3(C2)C(C)CCC3C1(C)COC(C)=O
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	43.07	kJ/mol	Joback Method
hf	-358.89	kJ/mol	Joback Method
hfus	21.16	kJ/mol	Joback Method
hvap	59.91	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.958		Crippen Method
mcvol	220.950	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	1833.00		NIST Webbook
tb	683.71	K	Joback Method
tc	903.97	K	Joback Method
tf	453.29	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.96	J/mol×K	683.71	Joback Method
cpg	689.22	J/mol×K	720.42	Joback Method
cpg	709.66	J/mol×K	757.13	Joback Method
cpg	729.52	J/mol×K	793.84	Joback Method
cpg	749.07	J/mol×K	830.55	Joback Method
cpg	768.58	J/mol×K	867.26	Joback Method
cpg	788.29	J/mol×K	903.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R199230&Units=SI

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