8 «alpha»,13-epoxy-14,15,16-trinorlabd-12-ene

Inchi: InChI=1S/C17H28O/c1-15(2)9-6-10-16(3)13(15)8-11-17(4)14(16)7-5-12-18-17/h5,12-14H
InchiKey: PTSWQZGZSZFGQN-YQEWQEHLSA-N
Formula: C17H28O
SMILES: CC1(C)CCCC2(C)C1CCC1(C)OC=CCC12
Mol. weight [g/mol]: 248.40

Physical Properties

Property code	Value	Unit	Source
gf	125.96	kJ/mol	Joback Method
hf	-275.79	kJ/mol	Joback Method
hfus	16.14	kJ/mol	Joback Method
hvap	54.77	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.922		Crippen Method
mcvol	219.380	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
ripol	2302.00		NIST Webbook
ripol	2302.00		NIST Webbook
tb	647.42	K	Joback Method
tc	892.92	K	Joback Method
tf	408.12	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.43	J/mol×K	647.42	Joback Method
cpg	677.21	J/mol×K	688.34	Joback Method
cpg	701.77	J/mol×K	729.25	Joback Method
cpg	725.57	J/mol×K	770.17	Joback Method
cpg	749.09	J/mol×K	811.09	Joback Method
cpg	772.84	J/mol×K	852.00	Joback Method
cpg	797.27	J/mol×K	892.92	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=R411768&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