13-ethoxy-8 «alpha»,13-epoxy-14,15,16-trinorlabdane

Inchi: InChI=1S/C18H32O2/c1-5-19-16-10-7-13-14(20-16)8-9-15-17(2,3)11-6-12-18(13,15)4/h1
InchiKey: PHUXMFIYWAEFPU-KVODCKKVSA-N
Formula: C18H32O2
SMILES: CCOC1CCC2C(CCC3C(C)(C)CCCC23C)O1
Mol. weight [g/mol]: 280.45

Physical Properties

Property code	Value	Unit	Source
gf	-2.80	kJ/mol	Joback Method
hf	-522.01	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	59.95	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.771		Crippen Method
mcvol	243.640	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
ripol	2464.00		NIST Webbook
ripol	2464.00		NIST Webbook
ripol	2556.00		NIST Webbook
tb	688.65	K	Joback Method
tc	915.03	K	Joback Method
tf	412.72	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.09	J/mol×K	688.65	Joback Method
cpg	795.64	J/mol×K	726.38	Joback Method
cpg	821.00	J/mol×K	764.11	Joback Method
cpg	845.43	J/mol×K	801.84	Joback Method
cpg	869.19	J/mol×K	839.57	Joback Method
cpg	892.54	J/mol×K	877.30	Joback Method
cpg	915.73	J/mol×K	915.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R344024&Units=SI
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

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